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NASA Technical Memorandum 4469

Microgravity Science and Applications

Program Tasks and Bibliography for FY 1992

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NASA Office of Space Science and Applications
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APPENDIX

I. Introduction

- Objectives and Focus for FY1992
- Program Research Task Summary Data

OBJECTIVES AND FOCUS FOR FY1992

NASA's Microgravity Science and Applications (MSA) Program reflects, as its over-arching purpose, a long-term commitment to the study of gravity-dependent phenomena—or those phenomena obscured by gravity—in a low- or *micro*gravity (μg) environment. In addition, the program seeks to focus on the use of space as a laboratory by undertaking the study of important physical, chemical, and biochemical processes on orbit that cannot easily be studied in the terrestrial gravity environment.

A microgravity environment affords unique characteristics that allow the investigation of phenomena and processes that are difficult or impossible to study on Earth. Significant reductions in critical characteristics, such as tension-driven buoyancy forces, convection, sedimentation and hydrostatic pressures, make it possible to isolate and control gravity-related phenomena and make measurements that generally have significantly greater accuracy than can be achieved in normal gravity. Space flight therefore gives scientists the opportunity to study, as never before, the fundamental states of physical matter—solids, liquids and gasses—and the forces that affect them. Because microgravity is the virtual absence of gravity as we know it, research in microgravity leads to a greater understanding, fundamentally, of the influence of gravity on the world around us. The results therefore lead to advances in knowledge and technologies that benefit both the sciences and their applications on Earth, while providing the practical knowledge essential to the development of future space systems.

The Office of Space Science and Applications (OSSA) is responsible for planning and executing research stimulated by the Agency's broad scientific goals. OSSA's Microgravity Science and Applications Division (MSAD) is responsible for guiding and focusing a comprehensive MSA program, and currently manages its research and development tasks through four major scientific disciplines: biotechnology, combustion science, fluid physics, and materials science.

The fiscal year 1992 was a notably active year for microgravity science in general and for MSAD in particular. Not only was an extensive ground research program maintained, there were also a total of three major Spacelab-based microgravity science missions flown aboard Space Shuttle orbiters during FY1992. The first International Microgravity Laboratory (IML-1) mission was flown in January 1992, and the first United States Microgravity Laboratory (USML-1) was launched in June to complete the longest Space Shuttle mission yet. For the third Spacelab mission in FY1992, MSAD flight hardware and personnel supported the Japanese Spacelab (SL-J) mission in August, which was dedicated to microgravity and life sciences. The first United States Microgravity Payload (USMP-1) was MSAD's fourth and final major mission in 1992. USMP-1 carried a set of ground-tended experiments—mounted on an exposed cargo bay support structure—into orbit in October.

This document, The Microgravity Science and Applications Program Tasks and Bibliography for Fiscal Year 1992 (October 1991 – September 1992), includes research projects now being funded by the Office of Space Sciences and Applications, Microgravity Science and Applications Division. The document is published annually and is sent to scientists in the field, both foreign and domestic. The information it contains is utilized in reports to the Associate Administrator, the Office of Management and Budget, and to the Congress.

The Microgravity Science and Applications Division wishes to thank The Bionetics Corporation, and in particular Ms. Celia Griffin and Mr. Duke Reiber, for their efforts in the compilation, development, and publication of this report.

FY1992 PROGRAM RESEARCH TASK SUMMARY: Overview Information and Statistics

Total Number of Principal Investigators: 144

Total Number of Publication Citations and Presentation Credits: 559

Total Number of Patents Cited: 7

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Number of Graduate Students Funded: 246

Number of Degrees Granted: 61

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FY1992 Mircrogravity Science & Applications Budget: .... $120.8 Million

Number of States with Funded Research (including District of Columbia): 32

Distribution of Microgravity Science & Applications Research Tasks and Types

Centers, Types of Research	Ground	Flight	ATD	Center Totals
Jet Propulsion Laboratory	13	4	2	**19**
Johnson Space Flight Center	2	1	0	**3**
Langley Research Center	4	1	1	**6**
Lewis Research Center	45	19	5	**69**
Marshall Space Flight Center	19	18	2	**39**
NASA Headquarters	8	0	0	**8**
Research Type Totals	**91**	**43**	**10**	**144**

II.
Microgravity Science & Applications Program Tasks for FY 1992

TYPE: Flight
DISCIPLINE: Biotechnology
PROJECT TITLE: *Electrophoretic Separation of Cells and Particles from Rat Pituitary and Rat Spleen*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-23-01-01

PRINCIPAL INVESTIGATOR: Dr. Wesley C. Hymer
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MAILING ADDRESS: Department of Microbiology
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TASK OBJECTIVE/DESCRIPTION

This experiment is designed to probe the mechanism by which the biological activity of pituitary hormones (growth hormones and prolactin) may be modified by exposure to microgravity.

RESEARCH APPROACH

The objectives are to separate pituitary cells as well as pituitary, hormone-containing granules by free-flow electrophoreses, using the Japanese Free-flow Electrophoresis Unit (FFEU). To accomplish these aims it is necessary first to optimize conditions for growing pituitary cells in the Japanese cell-cultural kits; second, remove cells from the growth chamber and fractionate them by electrophoresis; and third, lyse the cells grown in the chamber and fractionate the lysate to obtain the hormone-containing fractions. These procedures must be done in such a way as to be executable in flight. It is also necessary to develop the technologies to assay each sample and fraction for growth hormone, prolactin, and heat shock protein (HSP). The hormones will be assayed by immune and bioassays. A screen to detect the HSP immunocytochemically will be developed. Because of limited sample size and because of the buffers required for electrophoresis, procedures used routinely for ground-based research must be modified.

PROGRESS DURING FY1992

In order to be able to separate pituitary cells and their hormone-containing granules by electrophoresis in microgravity, it is necessary to use a specially developed cell chamber and free-flow electrophoresis unit developed by the Japanese Space Agency for this experiment. In 1992 we established that several of the cell procedures could be used. We were also able to do a limited number of runs with the FFEU unit, which is in Japan.

We established that the cells can be lysed in buffer compatible with electrophoresis and that lysate can be concentrated and separated on the FFEU. Growth hormone and prolactin were each assayable by at least one assay. We also established that

pituitary cells could be maintained and recovered from a chamber similar to that to be used with the FFEU. We also found that the culture medium will have to be modified to be compatible for bioassays and electrophoresis as well as for growth.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Mukherjee, P., and Hymer, W. C. Heterogeneity of rat pituitary prolactin cells: Relationships among location, hormone assay and estrous cycle stage. *Neuroendocrinimmunology, 5*, 108–119, (1992).

— Mukherjee, P., Houser, U., and Hymer, W. C. PRL-immune interactions in breast cancer. *Journal of Cell Biology 115,* 78a (1991) .

— Mukherjee, P., Epp, L., Viselli, S., Mastro, A. M., and Hymer, W. C. PRL cell function in the individual rat pituitary gland in vitro: Importance of physiological state of the donor. Presented at the 74th Annual Meeting of the Endocrine Society, 1992.

— Viselli, S., and Mastro, A. M. PRL receptors are found on a heterogeneous subpopulation of rat splenocytes. *Endocrinology.* In press, 1992 .

TYPE: Flight
DISCIPLINE: Biotechnology
PROJECT TITLE: *Enhanced Hybridoma Production Using Electrofusion*
RESPONSIBLE CENTER: JSC **PROJECT IDENTIFICATION:** 694-23-01-02

PRINCIPAL INVESTIGATOR: Dr. David W. Sammons
AFFILIATION: University of Arizona
MAILING ADDRESS: University of Arizona
Center for Separation Science
Bldg. #90, Rm 211
Tucson, AZ 85721
PHONE: (602) 621-2157

TASK OBJECTIVE/DESCRIPTION

The objectives of the hybridoma flight are to determine the extent to which sustained microgravity environment increases electrofusion frequencies and hybridoma yields compared to ground-based controls, and secondly, to enhance working knowledge of lymphocyte activation and cell culture.

RESEARCH APPROACH

The hardware is being developed by Zimmerman et al., in Germany and furnished to Drs. Sammons and Neil under an international agreement. The NASA investigators will furnish B cells for activation and subsequent data analysis. Nonactivated, preselected B cells will be activated in flight and through a high-efficiency process fused to an SP2 cell line for the production of specific hybridomas. Typically, electrofusion protocols allow the generation of antigen-specific hybridomas with an efficiency of 1 in 10,000, using 106 SP2 cells in the profusion chamber. The object of this experiment is to identify the effect of microgravity on fusion frequency and specificity.

PROGRESS DURING FY1992

Investigators completed ground-based investigations and critical design review. The experiment is manifested for STS-55, which will fly in February 1993.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Biotechnology
PROJECT TITLE: *Electrophoresis Technology*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-23-08-04

PRINCIPAL INVESTIGATOR: Dr. Robert S. Snyder
AFFILIATION: NASA Marshall Space Flight Center (MSFC)
MAILING ADDRESS: Marshall Space Flight Center
Mail Code ES76
National Aeronautics and Space Administration
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PHONE: (205) 544-7805

TASK OBJECTIVE/DESCRIPTION

The task objectives are to study the effects of sample concentration and dielectric constant on sample stream distortion and the limits of the electrohydrodynamic stability of the sample stream in the absence of shear flow. Since the Continuous Flow Electrophoresis System (CFES) built by the McDonnell Douglas Astronautics Company achieved results in space on seven Shuttle missions that were influenced by electrohydrodynamics, these scientific phenomena are a critical part of electrophoresis in space. The severity of sample distortion due to dielectric constant variations is not known in the laboratory to date because of the concurrent sample concentration effect.

The electrophoresis separation process can be considered to be simple in concept, but flows local to the sample filament produced by the applied electric field have not been considered. These electrohydrodynamical flows, formulated by G. I. Taylor in 1965 for drops suspended in various liquids, distort the sample stream and limit the separation. In addition, electroosmosis and viscous flow, which are inherent in the continuous-flow electrophoresis device, combine to further disturb the process. Electroosmosis causes a flow in the chamber cross section which directly distorts the sample stream, while viscous flow causes a parabolic profile to develop in the flow plane. These flows distort the electrophoretic migration of samples by causing a varying residence time across the thickness of the chamber. Thus, sample constituents at the center plane will be in the electric field a different length of time and hence move more or less than comparable constituents closer to the chamber wall.

Both horizontal and vertical laboratory electrophoresis test chambers have been built to test the basic premise of continuous-flow electrophoresis that removal of buoyancy-induced thermal convection caused by axial and lateral temperature gradients will result in improved performance of these instruments in space. These gravity-dependent phenomena disturb the rectilinear flow in the separation chamber when high-voltage gradients and/or thick chambers are used, but

distortion of the injected sample stream due to electrohydrodynamic effects causes major broadening of the separated bands observed in these chambers.

RESEARCH APPROACH

The initial part of the proposed space experiment will be done in the French electrophoresis hardware (RAMSES) on the second International Microgravity Laboratory (IML-2). This hardware has the capability of applying the required voltage at 1,000 Hz, which will permit part of the dielectric dependency to be determined. d. Two different frequencies will be used to vary the dielectric constant of the samples. Samples will not be collected, but the cross-section illuminator will be used to show the sample filament cross section, and the observed shapes will be recorded photographically.

The higher frequency can be accommodated on a later RAMSES flight, or available TEXUS electrophoresis hardware, with its cross-section illuminator, can be supplied with the required high-frequency power supply. These measurements can then be completed during a short-duration rocket flight.

PROGRESS DURING FY1992

Most activities during FY92 have been directed toward adapting our requirements to the RAMSES design. The borate buffer preferred by the European principal investigators (PI's) is not optimum for our polystyrene latex samples. The cross-section illuminator will be a laser rather than single-filament lamp, and this also introduces problems of resolution. We are building a prototype chamber for conducting critical tests.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Low-Velocity, Opposed-Flow Flame Spread in a Transport-Controlled, Microgravity Environment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-02

PRINCIPAL INVESTIGATOR: Prof. Robert A. Altenkirch
AFFILIATION: Mississippi State University
MAILING ADDRESS: Mississippi State University
School of Engineering
P.O. Drawer PE
Mississippi State, MS 39762
PHONE: (601) 325-2270

TASK OBJECTIVE/DESCRIPTION

The objective of the work is to uncover the underlying physics of the mechanisms that cause flames to propagate over solid fuels against a low velocity of oxidizer flow in a low-gravity environment, where flame and fuel surface radiative effects and details of diffusional processes are important. Although the work is fundamental in nature, it has clear applications to fire safety in space and on Earth. Specific objectives are:

1. To analyze experimentally observed steady-flame shapes, measured gas-phase field variables, spread rates, radiative characteristics, and solid-phase regression rates for comparison with theoretical prediction capabilities; and

2. To investigate the transition from ignition to either steady-flame propagation or steady-flame extinction in order to determine the characteristics of those environments that lead to flame evolution to steady state.

RESEARCH APPROACH

To meet the objectives of this research program, a matrix of experiments has been developed to exercise several of the dimensional, controllable variables that affect the flame-spread process in microgravity. Those variables that will be changed from experiment to experiment are the opposing flow velocity, the external radiant flux directed to the fuel surface, and the oxygen concentration of the environment. The matrix is organized to contain the minimum number of experiments to be conducted in order to obtain the information needed to meet the scientific objectives. Experimental results will be compared with unsteady, computational modeling results that are able to track the flame from ignition onward. Through such comparisons, the physics important to the flame-spread process may be identified.

PROGRESS DURING FY1992

A Science Requirements Document was prepared, and experimental design has proceeded. Approaches to meeting most of the science requirements experimentally have been developed, along with a plan for conducting the experiments aboard sounding rockets. Two potential fuel radiant heaters have been identified and are being designed and tested. Flame visualization techniques that were chosen include infrared and visible intensified video imaging utilizing filters to identify particular species and color filters to construct a color image of the flame from the black-and-white video camera. Unsteady modeling efforts have progressed, and the capability to carry out computations from ignition to steady spread or extinction has been demonstrated for thick fuels with and without fuel surface radiation. Gas-phase radiation is currently treated in an approximate way with an energy loss term in the gas-phase equations in which a Planck mean absorption coefficient is specified as a parameter.

GRADUATE STUDENTS: 7 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Altenkirch, R. A., Bhattacharjee, S., Olson, S. L., and Sacksteder, K. "Opposed-flow flame spreading in reduced gravity." Presented by R. A. Altenkirch at the Second International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

— Altenkirch, R. A., Tang, L., Bullard, D. B., and Bhattacharjee, S. "Unsteady flame spread over solid fuels in microgravity." Presented by R. A. Altenkirch at the World Space Congress, Washington, D C, September 5, 1992.

— Bhattacharjee, S., Bhaskaran, K. K. and Altenkirch, R. A. "Effects of pyrolysis kinetics on opposed-flow flame spread modeling." Presented by S. Bhattacharjee at the ASME/AIChE National Heat Transfer Conference, San Diego, CA, August 8–12, 1992.

— Bhattacharjee, S., Seaton, D., and Altenkirch, R. A. "The role of kinetic, transport, and thermodynamic properties on flame spread over a thin solid fuel in an opposed flow environment." Presented by D. Seaton at the Western States Section of the Combustion Institute meeting, Berkeley, CA, October 12 –13, 1992, WSSCI Paper No. 92-107.

— Bullard, D. B., Tang, L., Altenkirch, R. A., and Bhattacharjee, S. Unsteady flame spread over solid fuels in microgravity. Submitted to *Advances in Space Research*, 1992.

— West, J., Bhattacharjee, S., and Altenkirch, R. A. "Investigation of controlling parameters in transition between thermally thin and thermally thick flame spread over solid uels in an opposing flow." Presented by J. West at the Western States Section of the Combustion Institute meeting, Berkeley, CA, October 12–13, 1992, WSSCI Paper No. 92-106.

— West, J., Bhattacharjee, S. and Altenkirch, R. A. "Surface radiative effects on flame spread over thermally thick fuels in an opposing flow." Presented by J. West at the ASME/AIChE National Heat Transfer Conference, San Diego, CA, August 8–12, 1992. In preparation for Journal of Heat Transfer, 1992.

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Scientific Support for an Orbiter Middeck Experiment on Solid Surface Combustion*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-01

PRINCIPAL INVESTIGATOR: Prof. Robert A. Altenkirch
AFFILIATION: Mississippi State University
MAILING ADDRESS: College of Engineering
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Mississippi State, MS 39762
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TASK OBJECTIVE/DESCRIPTION

The objective of this project is to determine the mechanisms of flame spreading over solid fuels in the absence of buoyancy or other externally imposed flows.

This project is the first combustion space experiment in the microgravity program and consists primarily of a series of eight flights of the Solid Surface Combustion Experiment (SSCE) aboard the Orbiter Middeck of the Spacelab Module.

RESEARCH APPROACH

In addition to the scientific support for the development of the SSCE flight hardware, flight operations, and postflight data analysis, this project is developing a highly complex computational model of opposed-flow flame spreading. The model includes detailed heat transfer mechanisms, most notably a model for radiative interactions throughout the gas phase (including the flame) with both the surroundings and the fuel, and chemical models for both the fuel pyrolysis and flame kinetics.

PROGRESS DURING FY1992

During this year the fourth and fifth flights of the SSCE were completed. These flights constitute the final flights of the thermally thin, ashless filter-paper samples.

Two significant extensions to the ongoing numerical modeling effort were accomplished this year. A time-varying code was evolved from the previously steady model in order to account for unsteady ignition effects and for the effects of boundary layer development over finite length samples in opposed flows. To account for differences between flame shapes observed in the flight experiment and those computed in the simulation, an extension to the numerical domain was created that permits the diffusion of species behind the flame.

Extensive effort was expended on the computational effort to simulate the pressure effects on flame spread rates observed in the SSCE flight experiments. It was shown that without the comprehensive gas-phase radiation aspect of the model, these pressure influences are not predicted.

GRADUATE STUDENTS: 2   **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Altenkirch R. A., Bhattacharjee, S., Olson, S. L., and Sacksteder, K. "Opposed-flow flame spreading in reduced gravity." 2nd International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

— Bhattacharjee, S., and Altenkirch, R. A. A comparison of theoretical and experimental results in flame spread over thin condensed furls in a quiescent, microgravity environment. *Proceedings of the Twenty-fourth Symposium (International) on Combustion, Sydney, Australia.* In preparation, 1992.

— Bhattacharjee, S., Altenkirch, R. A. , and Sacksteder, K., Implications of spread rate and temperature measurements in flame spread over a thin fuel in a quiescent, microgravity, space-based environment. In preparation for *Combustion Science and Technology,* 1992.

— Bullard, D. B., Tang, L., Altenkirch, R. A., and Bhattacharjee, S. "Unsteady flame spread over solid fuels in microgravity." Presented at the 1992 World Space Congress, Washington, DC. Submitted to *Advances in Space Research, COSPAR., 1992.*

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Gas Jet Diffusion Flames (GDF) Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-03

PRINCIPAL INVESTIGATOR: Dr. Yousef Bahadori
AFFILIATION: SAIC, Inc.
MAILING ADDRESS: Science Applications International Corporation
Thermal Hydrodynamic Division
21151 Western Avenue
Torrance, CA 90501-1724
PHONE:

TASK OBJECTIVE/DESCRIPTION

The overall objective is to improve our fundamental understanding of gas-jet diffusion flames in the laminar, turbulent, and transition regimes. Specifically, tests are to be conducted in microgravity with the purposes of (a) determining the effect of buoyancy on these flames, (b) determining the relative importance of buoyancy-induced turbulence on flame characteristics, and (c) revealing phenomena which may be masked by buoyant convection.

RESEARCH APPROACH

Measurements will be obtained from low-gravity (and counterpart normal-gravity) experiments and will be used to validate theoretical models of gas-jet diffusion flames. In this way, the mechanisms controlling the observed phenomena may be identified. The measurements include temperature, thermal radiation, pressure, species concentration, acceleration, and a record of the flame's appearance (through photography). Reduced-gravity tests will be conducted in the 2.2-second drop tower, zero-gravity facility, KC-135 aircraft, and in space as required. The past focus of the research was on laminar flames, while the current focus is on high-momentum flames, particularly in the laminar-to-turbulent transition regime.

PROGRESS DURING FY1992

Contract NAS 3-25982 was initiated in November 1991, replacing the previous contract and combining elements of the laminar flames program with the new high-momentum flames program.

In support of the laminar flames study, tests were conducted on the KC-135 in December 1991. In general, the flames showed the same characteristics observed in tests in the zero-gravity facility. However, they were strongly disturbed by the g-jitter on the aircraft. In some tests, the experiment package was floated within the aircraft. In this configuration, the flames were relatively steady until the package struck the wall. The float time was 8 seconds on average (i.e., close to the 5 seconds available in the zero-gravity facility). These results were presented in a poster

session at the Spring Technical Meeting of the Central States Section of the Combustion Institute, in Columbus, Ohio.

No tests were conducted in the zero-gravity facility during this period, due to the facility shutdown; the laminar flames tests planned for this facility have yet to be completed.

A space experiment for the laminar flames program was formally proposed at a CoDR in December 1991, where it was rejected. The PIs were directed to submit a proposal in response to the next NRA if they wanted to repropose the experiment.

L. Zhou, a postdoctoral student from the University of California at Berkeley, moved to NASA LeRC in March 1992 to perform research in support of the high-momentum flames research. L. Zhou and D. Vaughan (an undergraduate) conducted microgravity tests in the drop tower from the laminar to turbulent range, with a variety of hydrocarbon fuels. The experimental results have shown that the transition to turbulence is clearly different in microgravity and normal gravity. In the microgravity flames, the disturbances propagate upward from the base of the flame, whereas in normal gravity the disturbances first occur at the tip of the flame. This and other results have generated a great deal of interest at the technical meetings where the research has been presented.

Y. Bahadori and U. Hegde submitted a Glovebox-2 proposal using a disturbed laminar flame to study the vortices which naturally occur in the transition-regime flames. This proposal was accepted for USML-2, but the PIs and NASA LeRC are also considering the benefits of conducting this experiment in GAS Can hardware similar to that designed for the Fernandez-Pello's smoldering combustion experiment. A CoDR for this disturbed-flame experiment is planned for mid-1993.

In support of this proposed space experiment, 2.2-second drop tests have been conducted with a flame-disturbance mechanism proposed by D. Vaughan. The preliminary tests have shown that this mechanism can produce the desired disturbances. Additional microgravity testing is planned for FY93, including some tests with an alternate flame-disturbance mechanism.

Work continued on the numerical modeling of the laminar flames, and included an inhouse presentation of results (May 1992). An analytical model of the effect of buoyancy and axial diffusion on confined diffusion flames (i.e., Burke-Schumann flames) was developed by Hegde and Bahadori. The model predictions correlate well with measurments from Stocker's 2.2-second drop tests. Plans have been made by Bahadori and Hegde for analytical and numerical modeling to be conducted in FY93 in support of the proposed disturbed flame experiment and the high-momentum flames research in general.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Bahadori, M.Y., and Edelman, R. B. Combustion of gaseous fuels under reduced-gravity conditions. Paper LB-038, *Proceedings of the Second Symposium on Lunar Bases,* Lunar and Planetary Institute, Houston, Texas, in press., 1992.

— Bahadori, M. Y., Edelman, B., Stocker, D. P., Sotos, R. G., and Vaughan, D. F., "Effects of oxygen concentration on radiative loss from normal-gravity and microgravity flames." Paper AIAA-92-0243, AIAA 30th Aerospace Sciences Meeting, Reno, NV, January 1992.

— Bahadori, M. Y., Stocker, D. P., Vaughan, D. F., Zhou, L., and Edelman, R. B., "Effects of buoyancy on laminar, transitional, and turbulent gas jet diffusion flames." Presented at the Second International Microgravity Combustion Workshop, Cleveland, OH, September 1992.

— Bahadori, M. Y., Vaughan, D. F., Stocker, D. P., Weiland, K. J., and Edelman, R. B., "Preliminary observations on the effects of buoyancy on transitional and turbulent diffusion flames." Presented at the 1992 Spring Technical Meeting of the Central States Section of the Combustion Institute, Columbus, OH, April 1992.

— Hegde, U., and Bahadori, M. Y. "Gravitational influences on the behavior of confined diffusion flames." Paper AIAA-92-0334, AIAA 30th Aerospace Sciences Meeting, Reno, NV, January 1992.

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Investigation of Laminar Jet Diffusion Flames in Microgravity: A Paradigm for Soot Processes in Turbulent Flames*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-04

PRINCIPAL INVESTIGATOR: Prof. Gerard M. Faeth
AFFILIATION: University of Michigan
MAILING ADDRESS: Department of Aerospace Engineering
218 Aerospace Engineering Building
University of Michigan
Ann Arbor, MI 48109-2140
PHONE: (313) 746-7202

TASK OBJECTIVE/DESCRIPTION

The project is an experimental and theoretical investigation of the mechanisms of soot formation in laminar jet diffusion flames under conditions of low buoyancy. The final objective is a flight experiment in the Combustion Experiment Module. These experiments, combined with ground-based low, and normal-gravity experiments, will increase the current fundamental understanding of soot formation processes in both laminar and turbulent flames. This will have a significant impact on understanding of the spread of unwanted fires, and on the design of jet engines and large-scale boilers.

RESEARCH APPROACH

Several types of experiments have been conducted. The majority have been in normal gravity, studying the influence of gravity by varying the ambient pressure. In addition, experiments have been conducted on NASA's low-gravity aircraft, (the KC-135 at JSC). The work has focused on mapping soot volume fraction, temperature, soot particle size and gas species in a variety of hydrocarbon flames. The flight experiment will be limited to measurement of soot volume fraction, soot particle size, and more limited temperature measurements. These experimental results, combined with theoretical modeling, will confirm or deny the applicability of the conserved scalar formalism to soot properties in diffusion flames.

PROGRESS DURING FY1992

Considerable progress has been made in both modeling and experiments. The program successfully passed CoDR in September 1992 and was approved to continue to RDR. These tests will consist of flames studies at a range of pressures and flow rates using the Combustion Experiment Module .

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

- Faeth, G. M., "Priorities for microgravity combustion research and goals for workshop discussions." Presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.
- Mortezavi, S., Sunderland, P., Jurng, J. J., and Faeth, G. M., "Structure and soot properties of non-buoyant laminar round-jet diffusion flames." Presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.
- Mortezavi, S., Sunderland, P., Jurng, J. J., and Faeth, G. M. "Structure of laminar buoyant jet diffusion flames at low pressure." Presented at the 1992 Spring Technical Meeting of the Central States section of the Combustion Institute.

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Fundamental Study of Smoldering Combustion in Microgravity***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-05

PRINCIPAL INVESTIGATOR: Prof. A. Carlos Fernandez-Pello
AFFILIATION: University of California, Berkeley
MAILING ADDRESS: Department of Mechanical Engineering
University of California-Berkeley
Berkeley, CA 94720
PHONE: (415) 642-6554

TASK OBJECTIVE/DESCRIPTION

The project is an experimental and theoretical investigation of the mechanisms of smoldering combustion in porous media, specifically in polyurethane foam. The final objective is a set of flight experiments in a GAS Can facility in the orbiter cargo bay. These experiments combined with ground-based low and normal gravity experiments will increase the current fundamental understanding of smoldering combustion, and this will have a significant impact on understanding of the initiation of unwanted fires both on the ground and in space.

RESEARCH APPROACH

Several types of experiments have been conducted. The majority have been in normal gravity, studying the influence of gravity by changing the direction of smolder propagation with respect to gravity. In addition, experiments have been conducted on NASA's low-gravity aircraft, (the KC-135 at JSC and the Lear Jet at LeRC). To date, the majority of the work has concerned one-dimensional configurations with the smolder front propagation tracked using thermocouples. Study of transition to flaming in three dimensional configurations has recently begun.

PROGRESS DURING FY1992

Considerable progress has been made in both modeling and experiments. The one-dimensional work was largely completed in 1992. Papers discussing the influence of gravity in these configurations will be submitted in FY 1993. The program successfully passed CoDR in December 1991 and was approved to continue to RDR with an initial test matrix of four tests. These tests will consist of two quiescent tests at different oxygen concentrations and two flow tests at different flow rates.

GRADUATE STUDENTS: 4   **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Fernandez-Pello, A. C., and Pagni, P. J. "A fundamental study of smoldering combustion in microgravity." Presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.

— Torero, J. L., Fernandez-Pello, A. C., and Urban, D. L. "Experimental observations of the effect of gravity changes on smoldering combustion." Poster presentation at the 24th International Symposium on Combustion, Sydney, Australia, July 1992.

— Torero, J. L., Kitano, M., and Fernandez-Pello, A. C. Opposed forced flow smoldering of polyurethane foam. Accepted for publication by *Combustion Science and Technology*, 1992.

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Premixed Laminar and Turbulent Flames at Microgravity***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-06

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TASK OBJECTIVE/DESCRIPTION

The objective of this work is to study the effects of gravity-induced buoyancy on the combustion limits of premixed gas flames. Four subtasks have been pursued:

1. Radiation effects on premixed gas flames;

2. Flame structure and stability at low Lewis number;

3. Flame propagation and extinction in cylindrical tubes; and

4. Experimental simulation of combustion processes using autocatalytic chemical reactions.

It is anticipated that the results of these studies will lead to an improved understanding of the fire hazards that may exist in orbiting spacecraft and of ways to minimize these hazards. Furthermore, such studies may lead to an improved understanding of the mechanisms of combustion limits in Earth-based combustion devices, which in turn could lead to the development of cleaner and more efficient engines through the use of lean premixed combustors.

RESEARCH APPROACH

For task 1, we are studying the effects of the addition of inert, radiant particles to gas mixtures to increase the absorption coefficient of the gas. This enables us to study both the optically thin and optically thick radiation regimes in a single experiment. Drop towers are used to obtain microgravity (μg) conditions.

For task 2, we are studying flames in a variety of gas mixtures having low Lewis number (Le) in KC-135 aircraft tests. The goal of these studies is to determine under what conditions, if any, the instabilities which occur in low-Le mixtures may lead to the development of stable, stationary spherical flames called "flame balls."

For task 3, we have conducted experiments at Earth gravity on flame propagation in vertical tubes of varying diameter, at varying pressures and with mixtures having varying fuels, inerts, and Le, and have measured the flame propagation rates just inside the extinction limit (Sb,lim). Since this quantity is predicted by most relevant theoretical models, the relative importance of buoyancy, flame stretch, heat loss to the tube wall, radiation loss, etc., may be assessed.

For task 4, we have introduced the use of aqueous autocatalytic propagating chemical fronts (in particular, the arsenous acid-iodate system) for the experimental simulation of premixed combustion in nonuniform and unsteady flows. These fronts more nearly match the assumptions made by most relevant theoretical models that do gaseous flames; for example, constant density, constant thermodynamic and transport processes, and no heat losses. We have studied propagation in a Taylor-Couette (TC) flow, that is, in the annulus between two rotating concentric cylinders, and in capillary-wave (CW) flow in a thin layer of fluid in a vibrating dish.

PROGRESS DURING FY1992

For task 1, experiments have shown that at small particle loadings, burning rates are reduced, peak pressures in constant-volume combustion are lower, and thermal decay rates in the burned gases are increased. These results indicate that the significance of radiative loss is enhanced by the addition of particles to the gas. With sufficient seeding, the burning rates are practically the same as those found in particle-free mixtures, the peak pressures are comparable, and the thermal decay rate is smaller than in particle-free mixtures. All of these observations are consistent with the hypothesis that at sufficiently high particle loadings, radiation is reabsorbed within the combustible medium, and thus may not constitute a fundamental limit in very large systems.

For task 2, we have observed flame balls in all mixtures with sufficiently low Le and near flammability limits, independent of the chemical mechanism, which are stable for at least the 20 seconds of low-g available. The lean μg flammability limits are leaner than any which can be observed at Earth gravity. By comparison with analytical models, it has been concluded that radiation from the combustion products, along with diffusive-thermal effects in low-Le mixtures, is probably the stabilization mechanism which allows flame balls to exist at μg. The drift velocity which results from the finite g-levels in the KC-135 aircraft leads to the formation of two types of quasi-cylindrical flame structures. A flight experiment is under development to determine if the apparent stability of flame balls can be confirmed in experiments where both the duration of μg is long (unlike drop-tower experiments) and the quality is significantly better than that in aircraft tests.

For task 3, we have found that the characteristics of the limits can be described in terms of the effect of the Grashof number Gr ≈ gd^3/a^2on the limit Peclet number Pe ≈

S_b lim(d/a), where g is gravity, d the tube diameter and a the thermal diffusivity at room temperature. At low-Gr the results are consistent with theoretical predictions for flame extinguishment by conduction loss to the tube walls. At higher Gr, results are consistent with buoyancy-induced extinction mechanisms, in the upward propagating case Pe ~ $Gr^{1/2}$ and in the downward case Pe ~ $Gr^{1/3}$.

Because of the difference in extinction mechanisms, we have found that the flammability limit can actually be wider for downward propagation than for upward propagation. In the upward case, at Gr > 2.0 x 108 (corresponding to a pipe-flow Reynolds number of 2000) turbulent flow is exhibited; the flame behavior can be either flamelet-like or distributed-like depending on Gr and Le.

For task 4, we have found that in TC flows under conditions where the flow is essentially a linear array of steady vortices, the experimental values of the propagation rate agree well with a model we developed to describe the interaction of a propagating front with a one-scale flow field. In TC and CW flow characterized by a broad range of scales, at low turbulence intensities (u') our results agree with a model developed by Yakhot in 1988. At higher u, where the thin front is disrupted, a different type of model we developed, based on turbulent transport models in these flows, describes our results well. However, our results at small $U = u'/S_L$ are compromised by buoyancy effects, since even the very small fractional density change across the aqueous front leads to significant buoyancy influences because of the very low S_L. Space experiments would enable us to study the aqueous fronts at values of U accessible to gas combustion experiments and numerical simulations, enabling us to create a "bridge" between studies of fronts with and without substantial density changes.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Buckmaster, J. D., Joulin, G., and Ronney, P. D. Structure and stability of nonadiabatic flame balls: II. Effects of far-field losses. *Combustion and Flame 84*, 411–422 (1991).

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TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Flame Spread Across Liquids*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-07

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TASK OBJECTIVE/DESCRIPTION

For flame spread over liquid fuel pools, the existing literature suggests three gravitational influences: (a) liquid-phase buoyant convection, delaying ignition and assisting flame spread; (b) hydrostatic pressure variation, due to variation in the liquid pool height caused by thermocapillary-induced convection; and (c) gas-phase buoyant convection in the opposite direction to the liquid-phase motion. No current model accounts for all three influences. In fact, prior to this work, there was no ability to determine whether ignition delay times and flame spread rates would be greater or lesser in low gravity.

Flame spread over liquid fuel pools is most commonly characterized by the relationship of the initial pool temperature to the fuel's idealized flash point temperature, with four or five separate characteristic regimes having been identified. In the uniform spread regime, control has been attributed to (a) gas-phase conduction and radiation, (b) gas-phase conduction only, (c) gas-phase convection and liquid conduction, and most recently (d) liquid convection ahead of the flame. Suggestions were made that the liquid convection was owed to both buoyancy and thermocapillarity. In the pulsating regime, complicated flow structures have been observed in both the gas and liquid phases, with circulation around several centers; these flows were attributed to combined thermocapillary and buoyant effects.

Of special interest to this work is the determination of whether, and under what conditions, pulsating spread can and will occur in microgravity in the absence of buoyant flows in both phases. One possible mechanism for pulsating spread in microgravity is if the "premixed gas- diffusive burning" pulsations are due to periodicity between gas-phase conductive and liquid-phase convective control. A second possibility, which will be determined by these investigations, is whether pulsations may be induced in low gravity by the presence of slow, forced, gas-phase flow.

RESEARCH APPROACH

The approach we have taken to resolving the importance of buoyancy for these flames is (a) normal gravity experiments with advanced diagnostics, (b) microgravity experiments, and (c) numerical modeling at arbitrary gravitational level.

PROGRESS DURING FY1992

Normal-gravity flame spread tests were conducted inside a large metal glovebox, 1.2 m long x 0.8 m wide x 0.65 m high, which served to eliminate drafts from the room. Experiments on pool depth effects (where buoyancy might be expected to be important) were carried out between temperatures of 13 °C and 21 °C, at approximately 1 °C intervals. For pools of l-propanol at T_{Liq} = 17.3 °C, the 10 mm pool shows a slightly higher flame speed than the 5 mm pool (borne out in several runs), and both are well above that shown by the 2-mm-deep tray. Furthermore, at this temperature, which is approximately the transition temperature from uniform to pulsating spread, the shallow pool clearly shows regular pulsations, while the others show only small amplitude irregular variations in spread rate. In fact, we found definite, cyclic pulsations at temperatures as high as 18.4 °C for the 2 mm pools, which was thought to be above the transition temperature, but very uniform spread for the deeper pools. This difference in flame spread character with depth provides indirect evidence that there may be a weak liquid-phase flow at these conditions that produces pulsations in a shallow fuel layer but yields uniform spread in deeper pools.

Well into the pulsating region, at T_{Liq} = 14.1 °C, all three depths showed regular pulsations, and it is quite clear that the spread rate is dependent on pool depth. Again, the deeper pool shows a higher flame propagation rate, with the difference between 5 mm and 10 mm now somewhat enlarged compared to the 17.3 °C pool. Furthermore, it is clear that the pulsation wavelength is also strongly dependent on pool depth. Deeper pools exhibit much longer wavelength pulsations, in this case 4 pulsations over the 25-cm distance presented for the 10-cm-deep pool, compared to 13 for the 2-mm-deep pool.

The pool depth has a strong effect on the pulsation wavelength, but there is no easily discernible temperature dependence. The depth effect may be due to a limitation imposed by the bottom on the size of the liquid circulation zone that slightly precedes the flame leading edge. This zone cannot fully develop in the shallow pools, and the flame catches up more rapidly. Drag on the bottom may also slow down this flow during each cycle, leading to more frequent pulsations but a lower overall velocity. This explanation is consistent with numerical predictions of more frequent pulsations for increasing values of liquid viscosity and/or decreasing surface-tension coefficient. For the 2-mm-deep pool, surface deformation may also be significant and lead to the formation of roll cells; these cells could be the cause of

the depth effect on pulsation. Future work is needed to resolve the subsurface flow in shallow fuel pools and to confirm this hypothesis.

Recently we examined the temperature field using rainbow schlieren deflectometry (RSD) and the velocity field using particle image velocimetry (PIV) for uniform and pulsating flame spread using propanol and butanol as fuels. These techniques had not been previously applied to this flame-spread problem. The RSD and PIV were recorded with standard CCD video cameras and S-VHS video recorders. The particle tracks, obtained using an 840-nm laser diode light sheet and 12 micron pliolite particles, were digitized, color coded, and time-averaged on the video record to assist analysis. The flow penetrates to the full depth of the pool, unlike the temperature field. Thus, as might be expected, the use of methods responding to thermal variations, such as RSD or interferometry, to infer the flow patterns, can be misleading.

No microgravity experiments were performed in FY92 because the Zero Gravity Facility at NASA Lewis was closed.

Our recent computational studies have addressed unsteady, axisymmetric and planar open pool configurations. The transient numerical model uses the SIMPLE algorithm with the SIMPLEC modification. This method uses primitive variables (u, v, p, h), a staggered mesh, and the hybrid-differencing scheme. The continuity equation is satisfied by solving the pressure-correction equation in the SIMPLE algorithm. A "phase-split" solution technique is used in that the gas and liquid phases are solved separately. The effects of blackbody radiation, surface tension, gravity level, variable density, and thermophysical properties, vaporization, and finite-rate chemical kinetics are included in the computational model. Infinitely fast chemical kinetics (i.e., the flame sheet approximation) cannot be assumed because the flame leading edge is premixed. The model assumes that the liquid surface remains flat and horizontal at all gravity levels. Solutocapillary forces and recession of the liquid surface due to vaporization are neglected. It is predicted that at normal gravity, the temperatures in the reaction zone are generally higher and the reaction zone thinner than at microgravity. The flame standoff distance is slightly smaller at normal gravity than at microgravity, but the reason for this is not as clear as with flame spread over solids. Without the effects of surface tension, flame-spread rates decrease with increasing gravity level. When surface tension is included, flame propagation is either uniform or pulsating depending on the gravity level and initial pool temperature.

Pulsating spread of the precursor flame in front of the main body of the diffusion flame is shown to be caused by the formation of a recirculation cell in the gas phase in front of the flame leading edge. This recirculation cell is formed by a combination of opposed flow in the gas phase due to buoyancy and concurrent flow in the liquid phase due to thermocapillary forces. At microgravity, a recirculation cell may still form in front of the flame leading edge solely due to the surface-tension-driven

shear flow. However, the strength of this recirculation cell is relatively weak compared to that at normal gravity. Therefore, periodic flame pulsations are not predicted at microgravity.

Hot gas expansion plays a significant role in the flame pulsation process by causing the periodic destruction of the gas-phase recirculation cell. Large hot gas expansion velocities oppose the flow of fresh oxygen to the reaction zone. Both a lack of oxygen due to the hot gas expansion and quenching by the liquid surface leads to the extinguishment of the precursor flame. When hot gas expansion is not included in the simulations, small backward and forward pulsations of the precursor flame still occur at normal gravity owing to the presence of the recirculation cell in front of the flame leading edge. However, the recirculation cell structure remains intact throughout the pulsation cycle, and the precursor flame is extinguished because of quenching by the liquid surface.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Miller, F. and Ross, H. Further Observations of flame spread across laboratory-scale alcohol pools. *Proceedings of the 24th International Symposium on Combustion, Sydney,* Sydney, Australia, 1992.
— Ross, H. Ignition of and flame spread across laboratory-scale pools of pure liquid fuels. Submitted to *Progress in Energy and Combustion Science,* 1992.
— Schiller, D. N. "Combustion above liquid fuel pools: buoyant and surface-tension-driven flow computations." PhD. dissertation, University of California, Irvine, CA. 1992.
— Schiller, D. N. and Sirignano, W. A. "Ignition and flame spread above liquid fuel pools." Paper WSCI-91-96, fall meeting of the Western States section of the Combustion Institute, 1992.

TYPE: Flight
DISCIPLINE: Combustion Science
PROJECT TITLE: *Scientific Support for a Space Shuttle Droplet Burning Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-22-05-03

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TASK OBJECTIVE/DESCRIPTION

The objective of this research effort is to provide scientific support, in collaboration with Professor F. Dryer of Princeton University, for a droplet burning experiment to be performed on board a space platform, This support will include performance of theoretical analyses relevant to the experiments, execution of drop-tower experiments to acquire additional data, analysis of experimental data obtained in ground-based experiments, and identification of test conditions for experiments in space. The overall objective of the research is to achieve fundamental advances in the science of droplets.

RESEARCH APPROACH

The objectives stated above will be pursued through the use of the 2.2-second drop tower with measurements made on heptane and methanol burning in atmospheres of normal air and in diluted atmospheres and through the analysis of data from this tower, and also from the S-second drop tower with these fuels as well as decane. The data will be analyzed for droplet diameter and extinction diameter by use of high-precision analysis systems. Flame diameters also will be obtained by suitable digital image analysis procedures.

The theoretical approach will employ asymptotic methods to relate observed extinction conditions to elementary rate parameters. Treatment of the data by use of the theory will help to identify experiments that need to be done in space. Additional experiments will also be performed to address the effects of relative droplet-gas convection on burning rates. In the theoretical part of the project, a spherosymmetric, time dependent, finite element-based numerical model with detailed gas phase kinetics, and variable property effects will be extended to study the effects of soot formation in droplet burning. Extension of the existing one-dimensional code to two-dimensional axisymmetric geometry will be evaluated.

PROGRESS DURING FY1992

Significant progress has been made concerning the extinction of heptane diffusion flames. Extinction diameters of heptane droplets were predicted by an asymptotic analysis that systematically reduced the chemistry to two-step, three-step, and four-step mechanisms. This reduction is not empirical or semi-empirical modeling, but instead is a logical reduction from underlying elementary rates of the multitude of steps involved. This is the first time that such a reduction has been accomplished for a fuel as complicated as heptane. The predicted extinction conditions are quite reasonable, but strongly dependent on fuel chemistry, and the magnitudes of uncertainties involved were estimated and shown to exceed a factor of ten for the extinction diameter. Necessary steps in improving the estimates were identified for future research. There is a possibility of a significant advance in understanding through this work.

A significant portion of the progress involves improvements to the numerical code to include soot shell formation due to the influence of thermophoretic effect and Stefan flow in droplet combustion and to include 92-step Warnatz kinetic mechanism for heptane. Some preliminary calculations were also carried out for methanol using a skeletal mechanism at different ambient pressures.

During this reporting period, CoDR for the Droplet Combustion Experiment (DCE) was also completed in collaboration with NASA personnel.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Card, J. M. Asymptotic analysis for the burning of n-heptane droplets using a four step reduced mechanism. *Combustion and Flame,* 1992.

— Card, J. M., and Williams, F. A. Asymptotic analysis with reduced chemistry for the burning of n-heptane droplets. *Combustion and Flame,* 1992.

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— Cho, S. Y., Yetter, R. A., and Dryer, F. L. A computational model for one-dimensional mass and energy transport in and around chemically reacting particles, including complex gas-phase chemistry, multicomponent molecular diffusion, surface evaporation, and heterogeneous reaction. *Journal of Computational Physics,* vol. 102, no. 1 (September 1992).

— Choi, M. Y. "Droplet combustion characteristics under microgravity and normal gravity conditions." Ph.D. dissertation, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, 1992.

— Choi, M. Y., Cho, S. Y., Dryer, F. L., and Haggard, J. B. Jr. Computational/experimental basis for conduction alkane droplet combustion experiments on space-based platforms. *Proceedings of the IUTAM symposium on microgravity fluid mechanics, Bremen, FRG.* H. J. Rath, ed. Berlin: Springer-Verlag, 1992.

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— Dryer, F. L. "Computational/experimental studies of isolated, single- component droplet combustion." Presented at the Second International Microgravity Combustion Workshop, NASA Lewis Research Center, Cleveland, OH, October 1992.

— Williams, F. A. "Studies of droplet burning and extinction." Presented at The Second International Microgravity Combustion Workshop, NASA Lewis Research Center, Cleveland, OH, October 1992.

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Directional Solidification of Cadmium Telluride*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-07

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TASK OBJECTIVE/DESCRIPTION

The objectives are to (a) calculate theoretical thermal and elastic stress fields for various orbital flight furnace/cartridge/ampoule/sample systems in order to minimize stress-producing defects, and (b) simulate the thermal and stress fields within ground-based and space-processed crystals, and to provide quidelines for fully analyzing and characterizing these flight crystals.

RESEARCH APPROACH

We will (a) develop of theoretical models of the directional solidification growth process to account for all of the relevant physics (b) verify these models with ground-based and space experiments to ascertain their validity; (c) modify and empiricised as necessary; (c) search the literature and conduct the tests necessary to provide the physical properties required by the model; and (d) simulate the directional solidification process and optimize the growth parameters, which will allow the grower to produce minimum-defect crystals.

PROGRESS DURING FY1992

1. Using experimental furnace wall temperatures, our thermal model predicted the magnitude of six thermocouples, which were installed on the ampoule in experiment NCZT05 (Grumman Corporation Research Center, Dr. David Larson) to within 4 °C over the entire several-day growth process.

2. We demonstrated that the ampoule-holder-support geometry and material have a large influence on interfacial growth velocity within the seed-transition region. Highly variable interfacial velocities are possible even when the ampoule pulling rate and furnace wall temperatures are constant.

3. Thermoelastic stress calculations have produced some valuable results that correlate with characterization data, including: a) the development of a Star-of-David stress pattern on the (111) plane wafers along with the resulting "W" stress pattern; b) the discovery of a nonlinearity in the furnace temperature profile,

for which a negative influence on the excess stress in the crystal was demonstrated; and c) demonstrated of the size of the region influenced by the end effect in the last-to-solidify region.

4. We surveyed and assessed the literature related to inelastic modeling and mechanical properties of DdTe. We initiated constitutive model development based on continuum slip concepts, the model by Haasen and co-workers, and experimental data in the literature. We developed a reliable numerical integration subroutine and implemented the model into a finite element code. Refinements and simulations are proceeding.

5. We initiated initial data-reduction and preliminary calculations of space-grown CdTe.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *GaAs Crystal Growth Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-21-05-02

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TASK OBJECTIVE/DESCRIPTION

The objective is to determine the magnitude of effects of buoyancy-driven convection on the crystal growth of bulk gallium arsenide (GaAs).

RESEARCH APPROACH

Selenium- doped (-10e-17) GaAs crystals are grown in controlled environments at selected environments affecting fluid flow: (a) low-gravity (minimal convection), (b) normal gravity a three separate orientations (vector stabilizing the temperature gradients, avector destabilizing the thermal gradient, and a vector transverse to the thermal gradient), and a magnetically damped flow (the three normal-gravity orientations with either axial or radial magnetic field). The distribution of dopant is measured and compared to numerical predictions. Selected electrical and chemical properties are measured and correlated with the dopant distribution. Both macro- and micro-segregation are determined.

PROGRESS DURING FY1992

We completed the second flight of the payload, prepared a preliminary report of results, and initiated a sample analysis. We also held a meeting of the joint Air Force-NASA contractor analysis team to discuss results and direction of characterization program and coordinated the move of PI from GTE Laboratories to Cleveland.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Compound Semiconductor Growth in Low-g Environment*
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** 694-21-06-01

PRINCIPAL INVESTIGATOR: Dr. Archibald L. Fripp
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to determine the effects of gravity-driven convection on the growth parameters and crystal properties of compound semiconductors.

The material chosen for study is the compound semiconductor alloy lead tin telluride. Lead tin telluride is a substitutional alloy of lead telluride and tin telluride that is miscible over the entire compositional range. The semiconductor properties of this material are dependent on the ratio of the two components, and consequently the uniformity of an array of devices is dependent on good compositional control.

This material was chosen for microgravity research because it is not only a useful semiconductor material which has been used for construction of infrared detectors and tunable diode lasers but also has a phase diagram similar to that of other compound semiconductors of interest, such as mercury cadmium telluride and mercury zinc telluride. Lead tin telluride is very interesting from a purely scientific point of view in that it is both solutially and thermally unstable, but in a one-dimensional analysis with growth axis parallel to the gravity vector, only one instability works, per orientation, at a time. This double convective instability cannot be made stable by balancing thermal and solutal expansion in a high-temperature gradient. This study will lead to a greater understanding of the effects of gravity-driven convection on the finished properties of this class of materials.

RESEARCH APPROACH

Lead tin telluride is amenable to study because it is easily compounded, it has a relatively low vapor pressure, it is single phase, and there is existing, though limited, literature on its growth and properties.

The desired growth mode is of course one in which convection is zero, so that compositional steady state can be reached. However, fluid dynamic calculations have shown that finite convection exists in the physical configuration used in crystal-growth experiments even at 1xE-8 Earth gravity if there is a density gradient orthogonal to the gravity vector.

However, due to the residual atmosphere the minimum gravity level expected on the Space Shuttle is roughly on the order of 1xE-7 Earth gravity. Hence experiments are designed such that interface movement, that is, growth rate, is greater that the anticipated fluid velocity.

PROGRESS DURING FY1992

Reportable progress in 1992 was primarily in the area of AADSF furnace calibration and in choosing the specific furnace parameters for the flight experiment. The conceptually simple task of furnace calibration had been hindered by damage to the sheathed thermocouples from the inconel muffle tubes and by the lack of a reliable value for the heat transfer coefficient between the muffle tube and the furnace wall.

The interaction between the muffle tube and the thermocouples and resultant damage to the thermocouples has been characterized. A new calibration sample has been designed that offers protection to the thermocouples. This sample has been used to calibrate the AADSF over a wide range of temperatures, pull rates, and insulation zone configurations.

The AADSF has been further calibrated and characterized by the growth of doped germanium with periodic interface demarcation and by the development of a heat transfer measurement device. This work provides the boundary conditions and measurement verification for subsequent numerical modeling.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Rosch, W., Jesser, W. A., Debnam, W., Fripp, A., Woodell, G., and Pendergrass, T. K. A technique for measuring the heat transfer coefficient inside a Bridgman furnace. Accepted by, *J. Cryst. Growth*, 1992.

— Rosch, W. , Fripp, A., Debnam, W., Simchick, R., and Sorokach, S. "Damage of fine diameter platinum sheathed type R thermocouples at temperatures between 950 and 1100°C." The 7th International Symposium on Temperature, Its Measurement and Control in Science and Industry, April 28–May 1, 1992, Toronto, Ontario, Canada. Accepted for publication in proceedings.

— Sears, B., Narayanan, R., Anderson, T. J., and Fripp, A. L. Convection of tin in a Bridgman system: Part I, Flow characterization by effective diffusivity measurements. Accepted by *J. Cryst. Growth*, 1992.

— Sears, B., Narayanan, R., Anderson, T. J., and Fripp, A. L. The detection of solutal convection during electrochemical measurement of the oxygen diffusivity in liquid tin. Accepted by *Metallurgical Transactions*, 1992.

— Sears, B., Narayanan, R., Anderson, T. J., Fripp, A. L., Debnam, W. J., and Woodell, G. A. Convection of tin in a Bridgman system: Part II, An electrochemical method for detecting flow regimes. Accepted by *J. Cryst. Growth*, 1992.

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— Tanveer, S. Convection effects on radial segregation and crystal melt interface in vertical Bridgman growth. Submitted to *J. Phys. Fluids A*, 1992.

— Wagner, C. , Friedrich, R., and Narayanan, R. Gravational effects and some extended results for bilayer convection of the Rayleigh Marangoni type. Submitted to *J. Phys. Fluids A*, 1992.

PATENTS — Fripp, Archibald L. "HTX, Heat Transfer Measuring Device." Patent application procedure started February 1992.

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *A Study of Solution Crystal Growth in Low-g*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-06

PRINCIPAL INVESTIGATOR: Dr. Ravindra B. Lal
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TASK OBJECTIVE/DESCRIPTION

The objective of this task is to grow crystals of triglycine sulfate in low-g and analyze or measure the effect of residual fluid motion on the growth rate.

The crystals' growth in the Fluid Experiments System will be measured or recorded on holograms. Fluid flow and growth rate will be measured postmission on reconstructed holograms.

RESEARCH APPROACH

An experiment entitled, "A Study of Solution Crystal Growth in Low-g" was flown on STS-42 on the First International Microgravity Laboratory (IML-1), January 22–29, 1992. Because of hardware problems, the TGS-2 run, in which a crystal of triglycine sulfate (TGS) was to have been grown for about 46 hours, was aborted. The TGS-1 run, where the major objective was to study the fluid motion and the effects of g-jitter by studying the motion of particles of three different sizes (199 μm, 468 μm, and 646 μm) in the fluid, was also not without problems. With the help of all the ground personnel in the Huntsville Operations Support Center (HOSC) and the crew, we were able to save the experiment to some extent. Data were recorded for particle motion with and without heating the growth cell. TGS crystal was grown for about 16 hours, and the particle motion data were recorded for the same period. This gave us the data for the particle motion with and without the crystal growth. In the first case we could see only the motion of particles owing to the variation of acceleration forces.

PROGRESS DURING FY1992

Preparation for IML-1 flight:

Many TGS seed crystals were grown by a low-temperature reciprocating solution growth technique. Seeds of proper orientation and sizes were selected from the above crystals for the flight and for ground control experiments. The selected seed crystals were analyzed at the Brookhaven National Laboratory for any defects, using

X-ray diffraction synchrotron radiation imaging technique. By this process we selected the seeds for the flight. The seeds were characterized for electrical properties.

IML-1 Flight:
The IML-1 mission was supported by Drs. R.B. Lal, A.K. Batra, W.R. Wilcox, J.D. Trolinger, and M.D. Aggarwal. Owing to the dedicated efforts of all ground personnel, including all NASA/MSFC and Teledyne Brown Engineering persons and the flight crew, the experiment was salvaged in part in spite of many hardware problems in the Fluid Experiment System (FES).

IML-1 Post Flight:
The space-grown crystal was retrieved from Edwards Air Force base in California by Dr. R. B. Lal.

An initial examination of the flight crystal from the TGS-1 run was carried out at Brookhaven National Laboratory using X-ray diffraction synchrotron radiation imaging, in collaboration with Dr. Bruce Steiner of National Institute of Standards and Technology (NIST). An examination of the entire uncut flight crystal indicates that the lattice orientation is uniform to 1-2 arc seconds locally and limited by the seed uniformity to 8 arc seconds for the entire crystal. This indicates extraordinary crystal regularity.

The flight crystal was cut at EDO/Barnes Engineering Division, Shelton, Connecticut, for detector fabrication, and a small piece was cut for X-ray diffraction imaging. Orientation of the cut edge of the crystal showed continuity between seed at the bottom and the space growth at the top, indicating a high degree of epitaxy of the space growth. The demarcation between the seed and the space growth is indistinct in the flight crystal; this demarcation is generally observed on ground owing to defects at the interface.

Polystyrene fluid flow markers that had been included in the space growth in the TGS-1 run are observed as small imperfections. All three different sizes of polystyrene particles are seen in X-ray diffraction images. We now have an operational particle-image motion-analyzing computer system in use to analyze images produced in the IML-1 space flight. Fluid motion is detected by tracking the particles from one hologram to the next. This is the first time a knowledge of g-variation in space shuttle will be determined by optical means. The theory of random inertial walk as predicted by Russian scientists will be tested. Preliminary observations show that the particles move in a random-walk type of process at typical velocities of about one micron per second. In the data so far, this random-walk process is dominant in the particle motion. We expect to encounter other cases where convection dominates. Some unusual phenomena have been observed. The particle motion does not behave as predicted by simple theories used so far. The relative velocities between small and large particles do not agree with

prior examinations; the small particles move faster than expected. Our observations suggest that a more general theory of inertial random walk will be required to explain this data.

The infrared detectors fabricated from the space crystal at EDO/Barnes Engineering Division have shown higher detectivity (D*) and responsivity than the ground crystal, but these have not reached the theoretical limit as expected.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Banan, M., Lal, R. B., and Batra, A. K. Modified triglycine sulfate (TGS) single crystals for pyroelectric infrared detector applications. *J. Mat. Sci, 27*, 2291–2297 (1992).

— Lal, R. B. "Growth of TGS crystal and the effect of g-jitter on particle motion aboard the IML-1 mission." Gordon Research Conference on Gravitational Effects on Materials Processes, Henniker, NH, July 18–23, 1993. In preparation, 1992.

— Lal, R. B. A study of solution crystal growth in low-g. NASA Technical Memorandum 4353, 193–201, 1992.

— Lal, R. B. "TGS crystal growth experiment on IML-1 mission." 44th International Astronautical Congress, Graz, Austria, October 16–22, 1993. In preparation, 1992.

— Lal, R. B., and Batra, A. K. Growth and properties of triglycine sulfate (TGS): A review. Invited review paper for a special issue of *Ferroelectrics* on crystal and crystal growth. In press, 1992.

— Lal, R. B., Batra, A. K., Wilcox, W. R., Trolinger, J. D., Steiner, B., and Witherow, W. K. "A study of solution crystal growth in low-g: An experiment on the First International Microgravity Laboratory (IML-1)." 10th International Conference on Crystal Growth, San Diego, CA, August 16–21, 1992.

— Lal, R. B., Batra, A. K.,Wilcox, W. R., Trolinger, J. D., Witherow, W. K., and Steiner, B. "Growth of triglycine sulfate sulfate crystals aboard First International Microgravity Laboratory (IML-1)." Sixth Annual Alabama Materials Research Conference, Auburn University, Auburn, AL, October 6–7, 1992.

— Sun, J. H., Carlson, F. M., and Wilcox, W. R. "Simulation of solution growth of triglycine sulfate growth in space." World Space Congress, Washington DC, September 1992.

— Sun, J., Carlson, F. M., and Wilcox, W. R. Simulation of triglycine sulfate crystal growth in space, *Microgravity* Q.2, no. 3, 159–168, 1992.

— Yang, L., Batra, A. K., and Lal, R. B. Growth and characteristics of triglycine sulfate (TGS) crystals grown by sting technique. *Ferroelectrics, 118*, 85–91, (1991).

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Orbital Processing of High-Quality Cadmium Telluride Compound Semiconductors*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-02

PRINCIPAL INVESTIGATOR: Dr. David J. Larson
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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to investigate the influence of gravitationally dependent phenomena on the growth and quality of cadmium zinc telluride (CdZnTe). The family of II-VI compound semiconductors, of which CdZnTe is a member, is used in the fabrication of nuclear detectors, gamma ray dectors, laser optics, electro-optic modulators, and infrared detectors. Orbital processing offers a unique opportunity to advance toward the goal of increased structural perfection within the bulk crystals and of more uniform specific lattice parameters within the substrate.

RESEARCH APPROACH

The CdZnTe samples will be grown in microgravity using the seeded Bridgman-Stockbarger method of crystal growth. Bridgman-Stockbarger crystal growth is accomplished by establishing isothermal hot-zone and cold-zone temperatures with a uniform temperature gradient between. The thermal gradient spans the melting point of the material (1,095 °C). After sample insertion, the furnace's hot-and cold-zones will be ramped to temperature establishing a thermal gradient of 25 °C/cm and melting the bulk of the sample. The furnace will then move farther back on the sample, causing the bulk melt to come into contact with the seed crystal, thus "seeding" the melt. The seed crystal prescribes the growth orientation of the crystal grown. Having seeded the melt, the furnace translation is reversed and the sample is directionally solidified at a uniform velocity by moving the furnace and the thermal gradient over the stationary sample.

PROGRESS DURING FY1992

Two CdZnTe samples were processed in the crystal growth furnace (CGF), which was flown in the pressurized Spacelab module in the habitable environment of the Space Shuttle Columbia during the first United States Microgravity Laboratory (USML-1) in June of 1992. The primary sample was processed for 92.5 hours and

approximately 10.6 cm of CdZnTe were grown. Processing of the second sample, at an abbreviated timeline, resulted in more than 2.8 cm of growth.

The two samples of CdZnTe are in the process of being examined using infrared and optical microscopy; microchemical analysis, X-ray precision lattice parameter mapping and synchrotron topography, and infrared transmission and optical reflectance. These characterization techniques will quantitatively map the chemical, physical, mechanical, and electrical properties of the flight crystals for comparison with identically processed CGF ground-processed samples. Based on the preliminary analyses, it can be concluded that the CdZnTe experiments have significance that greatly exceeds that which was anticipated. Each CdZnTe crystal experienced the predetermined temperature/time history, successfully seeded a monolithic single crystal, maximized the desired region of dewetting throughout the shouldering region, and demonstrated an unanticipated thermal and gravitational asymmetry throughout the steady-state growth period.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Crystal Growth of II-IV Semiconducting Alloys by Directional Solidification*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-04

PRINCIPAL INVESTIGATOR: Dr. Sandor L. Lehoczky
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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to investigate the effects of microgravity during the crystal growth of mercury zinc telluride (HgZnTe) on its compositional, metallurgical, electrical, and optical properties. The anticipated results of this study are both scientifically and technologically significant. The advancement in science will result from the increased understanding of the role of gravity on the fluid dynamic and compositional redistribution phenomena during the crystal growth of solid-solution semiconducting alloys having large separation between the liquids and solidus of the constitutional phase diagrams, and from the more accurate values of materials properties that can be measured using the high-quality, bulk crystals growth in space. Any advance in quality of these electronic materials has a great technological impact because of the application to infrared detectors for NASA and DOD requirements.

RESEARCH APPROACH

The HgZnTe alloy for this experiment will be prepared by reacting 99.9999+% pure, elemental constituents in evacuated, sealed, fused-silica ampoules. The HgZnTe will be agitated while molten to achieve complete reaction and homogenization, and then cast in the tapered end of an ampoule. The ampoule will then be installed in the hot zone of the growth furnace. The hot zone will be heated above the liquids temperature of the alloy, and the cold zone will be maintained at a temperature low enough to provide a gradient sufficient to prevent constitutional supercooling. The directional crystal growth will be accomplished by raising the temperature gradient through the ampoule. The crystal nucleates in the bottom tip of the ampoule and grows as the gradient is raised.

PROGRESS DURING FY1992

One HgZnTe sample was planned to be processed for approximately 148 hours in the crystal growth furnace (CGF), which was flown in the pressurized Spacelab module

in the habitable environment of the Space Shuttle Columbia during the first United States Microgravity Laboratory (USML-1) in June of 1992. Unfortunately, because of the loss of power to the CGF, the experiment terminated prematurely at about 39 hours into the experiment timeline. About a 5.5 mm sample was grown during this time period. The initial microstructural, compositional, and X-ray radiographic and diffraction results indicate that preprocessed alloy crystals can be successfully quenched, back-melted, and regrown maintaining nearly steady-state compositions. Further analysis of the sample is continuing.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: ***The Study of Dopant Segregation Behavior During the Growth of GaAs in Microgravity***
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-05-01

PRINCIPAL INVESTIGATOR: Dr. David H. Matthiesen
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TASK OBJECTIVE/DESCRIPTION

The objectives of this program are to investigate gravitational and thermal techniques for obtaining complete axial and radial dopant uniformity of the selenium dopant during crystal growth of gallium arsenide (GaAs). These techniques include controlling the thermal conditions to obtain a flat interface shape and a steady-state growth rate and, most importantly, growth in the microgravity environment afforded by the Crystal Growth Furnace (CGF) in the first United States Microgravity Laboratory (USML-1).

RESEARCH APPROACH

Crystals of GaAs, 16.5 cm long by 1.5 cm in diameter, will be supplied by GTE Laboratories to NASA for growth in CGF on USML-1. These crystals will be doped with selenium to approximately $1 \times 10^{17}/cm^3$. As supplied to NASA, these crystals will be hermetically scaled in a specially designed fused quartz ampoule. This ampoule will then be sealed into an experiment cartridge, which on orbit will be loaded unto the furnace system for growth. The large hot zone length of the CGF (20 cm) should allow, for the first time in microgravity, the achievement of steady-state growth rates. After flight, extensive characterization of the electrical and structural properties is planned.

PROGRESS DURING FY1992

Three ampoules containing GaAs have been tested at GTE Laboratories. In addition, two alumina thermal probes and three GaAs samples have been tested in the Ground Control Experiment Laboratory (GCEL). The GCEL contains a ground-based equivalent of the flight unit, which has been delivered to the Kennedy Space Center for integration into the United States Microgravity Laboratory.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Cadmium Telluride Microgravity Growth*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-08

PRINCIPAL INVESTIGATOR: Dr. Ratnakar R. Neurgaonkar
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TASK OBJECTIVE/DESCRIPTION

The objective of this program is to determine optimal Bridgman growth conditions for CdTe single crystals within the envelope of parameters established for the experiments in space. This study includes the improvement—due to microgravity—of dislocation density, stoichiometry, electrical, and optical properties of V-doped and undoped CdTe. It seeks to achieve this by growing near-perfect, single grain and [110]-oriented crystal boules. The crystal perfection and quality is being optimized using photorefractive and electrical measurement techniques. A parallel effort on other aspects of CdTe growth is being conducted at Grumman preparatory to space experiments, and procedures for microgravity experiments will be developed jointly with Grumman.

RESEARCH APPROACH

A systematic study of parameters influencing the grain-oriented growth of doped and undoped CdTe single crystals is being conducted using oriented seeds in a Bridgman furnace. KC-135 flights are used to collect data on microgravity effects that can be used to relate ground-based experiments to eventual experiments in space.

PROGRESS DURING FY1992

We have developed, using selected dopants, Bridgman-growth conditions suitable for the growth of both optical-quality and near single-grain CdTe single crystals. Nearly perfect [111]-oriented crystals of V- and Zn-doped CdTe single crystals have been obtained using the parameters proposed for the flight experiments. KC-135 flights have been used to verify effects of free fall on the growth. We plan to continue this method of testing microgravity growth procedures. Among several dopants explored for this growth, only Vanadium (V) and zinc (Zn) produced crystals of reasonable quality, and these doped crystals exhibited sufficiently high resistivity for photorefractive applications. Further optimization of both the dopants and the crystal growth conditions is underway.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Bennett, M. J. , Tsiveriotis, K., and Brown, R. A. Nonlinear dynamics in periodically repeated sets of directional solidification cells. *Physical Review B, 45,* 9562–9575 (1992).

— Brown, R. A. "Crystal growing systems." Invited paper at NATO meeting on Interactive Dynamics in Convection and Solidification, Chamonix, France, March 1992.

— Brown, R. A., Lee, T. C. J., and Tsiveriotis, K. Nonlinear dynamics near the onset of cellular growth during thin-film solidification of a binary allow: On the observability of weakly nonlinear states. *Interactive Dynamics in Convection and Solidification.* S. H. Davis, et al., eds., Amsterdam: Kluwer, pp. 69–72, 1992.

— Kim, D. H., and Brown, R. A. Modelling of transients in growth of H_gCdTe by the vertical Bridgman technique. *J. Crystal Growth, 114,* 411–434 (1991).

— Kyrilidis, A. , and Brown, R. A. "Ability of nonperturbative density functional theories to stabilize arbitrary solids." American Institute of Chemical Engineers, Los Angeles, November 1991.

— Kyrilidis, A. and Brown, R. A. "Density-functional thermodynamic perturbation study of Lennard-Jones solids." In *Computational Methods in Materials Science,* , vol. 278. J. E. Mark, M. E., Glicksman, and S. P. Marsh, eds., Materials Research Society, pp. 21–26, 1992.

— Kyrilidis, A., and Brown, R. A. Local thermodynamic mapping for effective liquid density-functional theory. *Physical Review A, 45,* 5654–5659 (1992).

— Kyrilidis, A., and Brown, R. A. On the ability of nonperturbative density-functional theories to stabilize arbitrary solids. *Physical Review A, 44,* 8141–8181 (1991).

— Lee, C. T., and Brown, R. A. "Spatiotemporal chaos near the onset of cellular growth during thin-film solidification of a binary alloy." NATO Meeting on Interactive Dynamics in Convection and Solidification, Chamonix, France, March 1992.

— Lee, C. T., Tsiveriotis, K., and Brown, R. A. Spatiotemporal chaos near the onset of cellular gwowth in thin-film directional solidification. *J. Crystal Growth, 121,* 536–542 (1992).

— Mehrabi, R., and Brown, R. A. "Nonlinear analysis of morphological interactions between flow and interface shape. NATO Meeting on Interactive Dynamics in Convection and Solidification, Chamonix, France, March 1992.

— Mehrabi, R., and Brown, R. A. Nonlinear analysis of morphological interactions between flow and interface shape in the directional solidification of a binary alloy. *Interactive Dynamics in Convection and Solidification.* S.H. Davis, et al., eds., Amsterdam: Kluwer, pp. 65–67, 1992.

— Tsiveriotis, K., and Brown, R. A. Boundary conforming mapping applied to computations of cellular solidification. *Inter. J. Numer. Meths. Fluids, 14,* 981–1003 (1992).

— Tsiveriotis , K., and Brown, R. A. "The role of codimension-two bifurcation in cellular pattern formation in directional solidification." American Institute of Chemical Engineers, Los Angeles, November 1991.

Type: Flight
Discipline: Electronic Materials
Project Title: *Double Diffusive Convection during Growth of Lead Bromide Crystals*
Responsible Center: LeRC **Project Identification:** 694-21-05-03

Principal Investigator: Dr. N. B. Singh
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Task Objective/Description

Lead bromide is a highly attractive material for acousto-optic devices. Hardening of the crystal by dilute doping has been evaluated to prevent damage caused by postprocessing operations. However, bulk doping is difficult to achieve due to thermal-solutal convection. It is proposed to test convection effects in normal and reduced gravity and relate the results to the growth of device grade crystals.

Research Approach

To achieve these objectives, crystal growth experiments will be conducted on Earth and in space. Measurements involving Rayleigh number as a function of aspect ratio, and radius of the growth tube to the length of the melt column, will be made.

Progress During FY1992

Minutes of the March 1992 Flight Science Readiness Review have been published. Dr. Singh is taking action based on the recommendations of the review.

Graduate Students: 0 **Degrees Granted:** 0

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Vapor Crystal Growth Studies*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-05

PRINCIPAL INVESTIGATOR: Dr. Lodewijk van den Berg
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TASK OBJECTIVE/DESCRIPTION

The objective of this task is to grow one or more mercuric iodide single crystals in low-g.

This task will evaluate whether crystal growth in low-g will result in fewer crystal defects because of elimination of irregular convection and stress of crystals weight that occurs in 1-g. This material is very soft at growth temperature.

RESEARCH APPROACH

A crystal will be grown in space. The structural quality and the electronic properties of this crystal will be determined. These physical properties will be compared with the same properties measured for crystals grown on the ground from the same material and under similar conditions. An attempt will be made to explain the differences in the measured values on the basis of gravity effects.

PROGRESS DURING FY1992

After extensive training of the flight crew and the ground support group of scientists, a single crystal was grown during the flight of IML-1 (January 1992). The structural quality of the crystal has been determined by means of gamma ray rocking curves. A measurement was made at different points over the length of the crystal.

The data shows that a low-angle grain boundary ($< 0\text{-}2°$) runs through the crystal which gives rise to two sets of diffraction peaks. The peak width at half maximum of the individual curves is less than 0.04°, which indicates a high structural quality. It should be emphasized that this technique using high-energy gamma rays probes the entire depth of the crystal (approximately 1 cm).

Future analysis of the crystal properties will be performed in FY93.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

- van den Berg, L. Presentation at CNES program review meeting on the advantages of crystal growth from the vapor, Toulouse, France, June 1992.

TYPE: Flight
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Vapor Transport Crystal Growth of Mercury-Cadmium Telluride in Microgravity*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-21-08-03

PRINCIPAL INVESTIGATOR: Dr. Heribert Wiedemeier
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are (a) the establishment of experimental trends for the relation between convective flow, mass flux, and crystal morphology, and (b) the identification of microgravity effects and crystal properties for the ternary semiconductor mercury cadmium telluride (HgCdTe). The lateral and axial compositional homogeneity (distribution) of the major and dopant components is expected to be more uniform for the space-grown epitaxial layers. The density of dislocations, of strain-induced defects, and possibly the number of inclusions are expected to be considerably reduced relative to ground-control specimens.

RESEARCH APPROACH

This experiment requires the hot zone to be 625 °C and the cold zone to be 455 °C. The total duration of the experiment is 16 hours. The ampoule assembly is designed to be 160 mm in length, 18 mm outer diameter, and about 31 grams total weight. A cadmium telluride single crystal and a sapphire disc are used for the epitaxial crystal growth as substrate and substrate support, respectively. Four time intervals are required for crystal growth, namely, heat-up, annealing, growth, and cool-down periods.

PROGRESS DURING FY1992

Two HgCdTe samples were processed in the crystal growth furnace (CGF), which was flown in the pressurized Spacelab module in the habitable environment of the Space Shuttle Columbia during the first United States Microgravity Laboratory (USML-1) in June of 1992. After return to MSFC, the ampoule/cartridge assemblies were examined by X-ray radiation. In both cases, the thermocouples were in the proper locations along the ampoules. The mechanical integrity of the fused silica ampoules was confirmed after their removal from the cartridge. Based upon visual inspection of the flight ampoules, the surfaces of the source materials in both ampoules showed some recrystallization, which is typical for these procedures and

conditions. The epitaxial layers grown on the substrates were nearly mirror smooth and show a high degree of spectral reflection. This reveals the very high surface quality of the layer. Under comparable ground conditions, the surfaces of the epitaxial layers typically show a wavy morphology. Based on this qualitative comparison, the surface morphology of the epitaxial layers grown in a microgravity environment demonstrates a significant improvement relative to ground specimens. In addition, the epitaxial layers grown during the USML-1 mission have a very homogeneous appearance with respect to their overall surface morphology. Further characterization and further analysis of these flight experiments are proceeding.

GRADUATE STUDENTS: 0		**DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Surface Controlled Phenomena*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-24-04-03

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TASK OBJECTIVE/DESCRIPTION

The objectives of this task were to prepare experiments and samples to be performed in the Drop Physics Module during the USML-1 mission, to assist the astronauts during the execution of those experiments, and to analyze the data and publish the results of the investigations.

The experiments study the surface properties of free drops. One set of investigations deals with how these properties change with time, and how they are changed by the addition of small amounts of surfactants. A second set studies the degree to which surfactants affect the coalescence of two similar drops.

RESEARCH APPROACH

This task is supported by laboratory experiments and theoretical studies as well as by the information obtained during the flight. Using ultrasonic levitators and/or neutrally buoyant systems, the behavior of small drops is being refined, which includes the viscosities and elasticities of the surface. The flight experiments provide spherical drops within a negligible host; these simplifications will permit the corroboration of the developed theory.

PROGRESS DURING FY1992

A subset of the planned experiments was performed during the USML-1 mission. In addition to the expected observations, a variety of unexpected acoustic and surface phenomena were recorded.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Min., S., Holt R. G., and Apfel, R. E. Simulation of drop dynamics in an acoustic positioning chamber. *J. Acoust. Soc. Am.*, 3157–3165, (1992).

— Tian, Y., Holt, R. G., and Apfel, R. E., Frequency of quadruple drops in an acoustic field. Accepted for publication, *J. Acoust. Soc. Am.*, 1992.

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Kinetics of Diffusional Droplet Growth*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-24-08-01

PRINCIPAL INVESTIGATOR: Dr. Donald O. Frazier
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TASK OBJECTIVE/DESCRIPTION

Ostwald ripening is the process by which larger droplets grow at the expense of smaller ones by diffusion of mass away from droplets below a critical radius toward ones above this critical size. The phenomenon is important in many disciplines. The flight objective is to determine droplet growth rate constants and changes in size distributions using optical techniques for recording droplet data with time.

RESEARCH APPROACH

A transparent model binary liquid/liquid miscibility-gap type solution is the system of choice for the flight. The experimental approach is to deploy a fixed array of droplets of one liquid phase into a cell filled with the conjugate phase. This approach will greatly reduce any residual gravity effects (from "g-jitter" or maneuvers) and eliminate the possibility of coalescence. Ground-based studies determine the experimental parameters required to maximize the amount of data on "pure" Ostwald ripening obtainable during the flight experiment. Such parameters as volume fraction of droplet phase, initial droplet number, droplet spacing and sizes, the time required for the experiment, and ideal concentrations for supersaturation and growth must be determined.

PROGRESS DURING FY1992

Observation of Ostwald ripening in an isopycnic mixture of succinonitrile and water over a period of about 4 months, using holography, revealed a decreasing droplet number. However, instead of the predicted scaling behavior, 1^{-1}, droplet number decay scaled with $1^{-0.83}$ at the experiment's conclusion. This result may have been because (a) a limited sample size yielded observation of local effects, (b) experiment time was too short to achieve the predicted asymptotic limit, or (c) behaviors unaccounted for in the governing equations, such as diffusive processes, yielded density gradients. A detailed assessment of these holographic data, using a much larger sample size, is in progress.

To analyze the kinetics of the ripening progress, materials property measurements must include interfacial tension, density, and viscosity as functions of temperature and composition. Densities and solution molalities were required to determine the partial molal volumes of solution components by an analytical application of the method of intercepts. Partial molal volumes are easily convertible to partial molecular volumes, necessary as input to the Gibbs-Kelvin equation. A forthcoming paper will incorporate these data to analyze a complete test of the Lifshitz-Slyozov-Wagner development, and to expand the discussion to include large volume fraction of discrete phases.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Rogers, J. R., Downy, J. P., Witherow, W. K., Fecermire, B. R., and Frazier, D. O. A study of Ostwald ripening of a liquid-liquid system using a holographic technique. Submitted to *Proceedings of Heat Transfer in Microgravity Systems; 1993 National Heat Transfer Conference, Atlanta, GA, August 8–11, 1993,* 1992.

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Geophysical Fluid Flow Cell*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-24-08-04

PRINCIPAL INVESTIGATOR: Dr. John E. Hart
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TASK OBJECTIVE/DESCRIPTION

The Geophysical Fluid Flow Cell Experiment (GFFCE) takes advantage of the unique environment of the microgravity laboratory, which permits forces that would otherwise be swamped by normal terrestrial gravity to become dominant. The geophysical fluid flow cell uses electrostatic fields to warp gravity into a radial vector field, centrally directed towards the center of the cell. This allows us to perform visualizations of thermal convection in a spherical shell of liquid subject to imposed differential heating and rotation, where the resulting buoyancy forces are radially directed.

This fundamental configuration is significant, because large-scale motions of the atmospheres of planets and many stars are strongly constrained by rotation, under the action of Coriolis forces, and by gravity, which is manifest in the buoyancy forces that drive thermal circulations. The GFFC experiments will provide fundamental laboratory data that can be applied to problems of jetstreams on the giant planets, differential rotation on the Sun, and motions in the Earth's core and mantle.

RESEARCH APPROACH

The research has two components: hardware development, and basic theoretical and numerical study of spherical convection in preparation for USML-2. A significant modification to the original GFFC experiment that flew previously on Spacelab-III is the addition of real-time video visualizations of the fluid turbulence that can be downlinked from the shuttle. This permits interactive experiments that can identify and focus on important flow regimes.

Theoretical and computational simulations of the expected flows are carried out in advance of the flight in order to suggest particular experiments that can critically advance our basic understanding. Such models usually involve various approximations or assumptions that must be checked experimentally.

PROGRESS DURING FY1992

The most exciting results are from a fully nonlinear computational model of thermal convection i the presence of strong basic rotation which varies with latitude. The resulting flows are composed of banana cells, as observed on the Spacelab-III flight of the GFFC, but the computation is simplified by using an approximation to the full sphere, the "equatorial annulus" geometry. The turbulence at high heating rates is found to be associated with extremely strong, even dominating, mean zonal jets.

A scaling of the model results with the observed heat flux of Jupiter, for example, loads to zonal jets with velocities of order 100 meters per second. This number is similar to Voyager observations. The turbulence can have isolated spots inbedded inthe self-induced zonal jets. When the basic rotation is sufficiently large the whole system pulsates. The resulting differential rotation and the turbulent convection pulses in almost-periodic bursts. If an effective eddy viscosity appropriate to solar convection is used, the pulsation period is about 13 years — nearly the observed period of the solar cycle. These model results suggest a new and potentially very important regime of convection that will be investigated by the GFFC on USML-2.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Interfacial Phenomena in Multilayered Fluid Systems*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-24-05-05

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TASK OBJECTIVE/DESCRIPTION

The main objective of the research is to design a three-liquid-layer flight experiment that will study the interaction of two interfacial tension forces of different magnitude and their effects on fluid flow in adjacent (outer) liquid layers. In addition, the mechanical coupling between the immiscible layers will be studied, and whether or not the convective flow in a liquid layer can be suppressed will be investigated. Finally, the conditions for the existence for oscillatory flow will be sought.

These results are expected to significantly advance our knowledge in the area of surface-tension-driven convection in multilayered fluid systems, and are, in addition, relevant to applications related to encapsulated float zone processing.

RESEARCH APPROACH

The general approach is to conduct ground-based normal-gravity testing and develop theoretical models of the combined buoyant convection-thermocapillary convection phenomena. The instrumentation and diagnostics are centered around the physics of interest; namely, flow fields, temperature fields, and interfacial shapes. The theories and numerical models developed and verified with the 1-g data will be used to design and predict the results of the flight experiment.

PROGRESS DURING FY1992

The Science Requirements Document (SRD) was finalized in preparation for the Science Review at LeRC in March 1992. Preparations were conducted for this review.

The principal investigator attended test container (TC) CDR in Friedrichshafen, Germany and reviewed the status of the TC design. Discrepancies between requirements and the design were documented as review item discrepancies (RIDs).

Work was successfully completed in formulating a one-dimensional model of a single layer representing the middle of the three-layer configuration. Knowledge gained here was incorporated into the three-layer models, and numerous test cases were run. Various fluid combinations were tested; FC-75 and silicone oil were selected as the flight fluids. Measurements were made at LeRC of the interfacial tension between FC-75 and silicone oil (for both 5 and 10 cS varieties) as a function of temperature.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Doi, T., and Koster, J. N. Thermocapillary convection in two immiscible liquid layers with free surface. *Phys. Fluids A., Fluid Dynamics,* submitted 1992.

— Fontaine, J. P., Koster, J. N., and Sani, R. L. Thermocapillary effects in a shallow cavity filled with high Prandtl number fluid. *Annales de Chimie—Science des Materiaux,* Masson, 1992.

— Koster, J. N., Prakash, A., and Fujita, D., "Bernard and Marangoni convection in immiscible liquid layers." ASME Meeting, San Diego, 1992; ESA Bruxelles Meeting, 1992.

— Koster, J. N., Prakash, A., Campbell, T. A., and Pline, A. "Analysis of convection in immiscible liquid layers with novel particle tracking velocimetry." ASME 1992 Winter Annual Meeting, November 8–13, 1992.

— Prakash, A., and Koster, J. N. Natural convection in three layers of immiscible liquid in a differentially heated shallow cavity. *Physics of Fluids A,* August 24, 1992.

— Prakash, A., and Koster, J. N. Natural and thermocapillary convection in three infinite layers of immiscible liquids. *European Journal of Mechanics B/Fluid,* June 18, 1992.

— Tong. W., and Koster, J. N. Interactive convection of water in a rectangular cavity including density inversion. *Numerical Heat Transfer,* July 31, 1992.

— Tong, W. and Koster, J. N. Penetrative convection in sublayer of water including density inversion. *Physics of Fluids A.,* June 1, 1992.

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Surface-Tension-Driven Convection Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-24-05-04

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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to further the understanding of the physical mechanisms associated with thermocapillary flow by (a) developing an accurate description of the physical mechanisms, (b) developing an accurate numerical mode, and (c) obtaining ground-based and flight experimental data to verify the physical mechanisms and the numerical model. The thermocapillary flows result from the fluid motions generated by the surface-tractive force that is caused by surface-tension variation due to the temperature gradient along the free surface.

RESEARCH APPROACH

The basis of the Surface-Tension-Driven Convection Experiment (STDCE) flight experiment is a copper test cell 10 cm in diameter and 5 cm deep, filled with silicone oil, to provide both a flat and curved free surface in a microgravity environment. The outer wall of the test cell is water cooled. The silicone oil can be centrally heated either externally by a carbon dioxide laser or internally by an immersion heater. The cross section is illuminated by a 1-mm-thick sheet of light, which scatters from small aluminum oxide particles mixed into the oil, allowing observation and measurement, using a particle-tracking technique, of the axisymmetric flow velocity. An infrared imager is used to measure surface temperature, and thermistors are used to measure fluid and wall temperature. The velocity and temperature measurements are compared with the numerical predictions.

PROGRESS DURING FY1992

The significant milestone was achieved with the successful completion of the STDCE during the USML-1 mission in July 1992. Thirty-eight tests of STDCE, operated for the first time in-orbit in Spacelab, were conducted in 12 1/2 hours to obtain thermocapillary flow data. The flight hardware provided better video flow data than expected, as well as infrared images, some of which were downlinked for observation and analysis by the PIs. Preliminary evaluation corroborates the

Principal Investigator's theory that oscillatory flows require lower viscosity liquids and smaller test chambers. Operations were controlled by a team of NASA Lewis Research Center engineers located in the Payload Operations Control Center at NASA's George C. Marshall Space Flight Center.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kamotani, Y., Lee, J. H., and Ostrach, S. An experimental study of oscillatory thermocapillary convection in cylindrical containers. *Phys. Fluids A4*, 955 (1992).

— Ostrach, S., Kamotani, Y., and Lee, J. "Oscillatory thermocapillary flows." Presented at the World Space Congress, Washington, DC, 1992.

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Thermocapillary Migration and Interactions of Bubbles and Drops*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-21-08-02

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TASK OBJECTIVE/DESCRIPTION

The objectives of the research are to experimentally measure the thermocapillary migration velocities and shapes of single and interaction gas bubbles and liquid drops in continuous phase under the action of an applied temperature gradient, and to compare the observed velocities and shapes with those predicted from theory.

These results are expected to advance our knowledge in the area of surface tension driven motion and are, in addition, relevant to several applications with respect to space processing of materials. Some examples of the latter include solidification, glass processing, and the preparation of composites.

RESEARCH APPROACH

The general approach is to conduct ground-based normal-gravity testing and develop theoretical models of the thermocapillary migration phenomena. The instrumentation and diagnostics are centered on the physics of interest; namely, flow fields, temperature fields, and bubble/droplet shapes. The theories and numerical models developed and verified with the 1-g data will be used to design and predict the results of the flight experiment.

PROGRESS DURING FY1992

The Science Requirements Document (SRD) was finalized in preparation for the Science Review at LeRC in March 1992. Preparations were conducted for this review.

The principal investigator attended test container (TC) CDR in Friedrichshafen, Germany and reviewed the status of the TC design. Discrepancies between requirements and the design were documented as review item discrepancies (RIDs).

Work continued on determining the dissolution rates of bubbles and droplets in silicone oil. It was determined that the changes in the bubble sizes were smaller for the time period tested (20 min); yet the methanol droplet tested underwent

significant changes in size. This was especially true for the smaller drops and/or at the higher temperatures.

Work is nearly completed on the interactions of two bubbles rising in a temperature gradient. Work also continued on the migration of methanol droplets in a temperature gradient. There were times for which it was difficult to demonstrate thermocapillary effects for these methanol drops on the ground. (Note: For the new drop fluid of choice, FC-75, strong thermocapillary effects are shown in the ground experiments.)

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Balasubramanian, R. and Dill, L. H. Thermocapillary bubble migration—an Oseen-like analysis of the energy equation. In *Microgravity Fluid Mechanics, IUTAM Bremen 1991,* H. J. Rath, ed. Berlin: Springer-Verlag, 1992, pp. 307–314.

— Dill, L. H. and Balasubramanian, R. Unsteady thermocapillary migration of isolated drops in creeping flow. *Int. J. Heat and Fluid Flow*, vol. 13, no. 1, pp. 78–85 (1992).

— Merritt, R. M., Morton, D. S., and Subramanian, R. S., Flow structures in bubble migration under the combined action of buoyancy and thermocapilarity. *J. Colloid Interface Sci.*, accepted for publication, May 1992.

— Merritt, R. M., Subramanian, R. S. Bubble migration under the combined actin of buoyancy and thermocapillarity. in *Microgravity Fluid Mechanics, IUTAM Bremen 1991,* H. J. Rath, ed. Berlin: Springer-Verlag, 1992, pp. 237–244.

— Nallani, M., and Subramanian, R. S., Migration of methanol drops in a vertical temperature gradient in a silicone oil. *J. Colloid Interface Sci.*, submitted for publication, June 1992.

— Rashidnia, N., Balasubramanian, R., and Del Signore, D. Interfacial tension measurement of immiscible liquids using a capillary tube. *AIChE J.*, vol. 38, no. 4, pp. 615–618, (1992).

— Subramanian, R. S., The motion of bubbles and drops in reduced gravity. Invited review in *Transport Process in Bubbles, Drops, and Particles* . R. P. Chhabra and D. De Kee, eds. New York: Hemisphere Publishing Corporation, 1992, pp. 1–42.

— Subramanian, R. S., Thermocapillary motion of bubbles and drops. In *Microgravity Fluid Mechanics, IUTAM Bremen 1991,* H. J. Rath, ed., Berlin: Springer-Verlag, 1992, pp. 393–403.

TYPE: Flight
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Drop Dynamics Investigation*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-24-04-01

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TASK OBJECTIVE/DESCRIPTION

The objective of this program is to understand the behavior of free drops, primarily by studying them in a microgravity environment. The Drop Physics Module (DPM) operated in the Space Shuttle provides an opportunity to address outstanding fluid-dynamics issues of rotating and oscillating simple and compound drops. To maximize the return from this short on-orbit opportunity, ground-based experiments will be performed to verify concepts and experimental techniques, and modeling will be done to select the parameters for the DPM experiments.

This investigation will use a triple-axis acoustic positioning chamber to study the static behavior and dynamics of simple and compound drops as well as of liquid shells. Equilibrium shapes and the stability of rotating and nonrotating drops, their associated internal flow patterns, and the centering force associated with shape oscillatory dynamics of rotating compound drops—will be the principal scientific areas of interest.

RESEARCH APPROACH

A variety of experiments will be performed in space. The most important of these is the study of oscillating drops—to verify the established models for small-amplitude behavior and to provide observations at large amplitudes to motivate improvements in the theory. Experiments to verify the location of the bifurcation point between the axisymmetric and two-lobed shape families for rotating drops will be performed and the dynamics of fission explored. The oscillation-mode spectrum of rotating drops will be measured for a variety of drop parameters. Compound drops and liquid shells will be formed to study their oscillation modes and their effectiveness between the acoustic field and the fluid will be studied: the drops' static shape, the stability of distorted shapes, and the generation of any flows in the liquid.

PROGRESS DURING FY1992

In preparation for the flight of USML-1, ground-based studies of drop stability when it is distorted by intense sound pressure were performed; a complementary theoretical study on bubble shapes was undertaken. Observations on the effects of relative size of two coalescing drops on their subsequent mixing were made and reported.

The flight of USML-1 provided several interesting results. Several high-quality runs to study the shape of drops in solid-body rotation were performed; these results are being submitted for publication. An unexpected torque caused the drops to rotate throughout the mission; the forced responses of the drops to oscillating acoustic pressure can be compared to existing theory. The ability of forced oscillations to center the inner fluid in a compound drop was demonstrated with both shells and two-liquid compound drops.

The anomalous torque is being investigated on the ground; it highlights the complexity of the acoustic-drop interactions inside the DPM.

GRADUATE STUDENTS: 6 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Anilkumar, A. V., Lee, C. P.. and Wang, T. G. Momentumless coalescence of drops." *AIAA paper No. 92-0111* (1992).

— Anilkumar, A. V., Lee, C. P., and Wang, T. G. Surface-tension-induced mixing following coalescence of initially stationary drops. *Phys. Fluids A, 3* , (11), 2587–2591 (1991).

— Lee, C. P., and Wang, T. G. Acoustic radiation force on a bubble. Accepted by, *JSA* , 1992.

— Lee, C. P., and Wang, T. G. Acoustic radiation pressure. Accepted by, *JSA* , 1992.

— Lee, C. P., Anilkumar, A. V., and Wang, T. G. The behavior of a liquid drop levitated and drastically flattened by an intense sound field. *AIAA paper No. 92-0112* (1992).

— Lee, C. P., Anilkumar, A. V., and Wang, T. G. Static shape and instability of an acoustically levitated liquid drop. *Phys. Fluid A* 3, (11), 2497–2515 (1991).

— Wang, T. G. Drop and bubble dynamics in the U.S. microgravity program. *AIChE Symposium Series 2833 87, National Heat Transfer Conference Proceedings,* S. B. Yilmas and B. G. Volintine, eds., Minneapolis, MN, 1991.

— Wang, T. G. Dynamics of free drops on USML-1. *IAF paper No. 91-399* (1991).

TYPE: Flight
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Modeling of Coalescence*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-24-05-02

PRINCIPAL INVESTIGATOR: Prof. Robert W. Gammon
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TASK OBJECTIVE/DESCRIPTION

The goal of the Critical Fluid Light Scattering Experiment (ZENO) is to measure the decay rate and correlation length of density fluctuations in xenon very near (1 K to 100 μK above) the liquid-vapor critical point in a low-gravity environment. Such experiments are severely limited on Earth because gravity causes a large density gradient in the fluid due to the divergence of the fluid compressibility as the critical temperature is approached. The data from this experiment will provide a test of critical phenomena theories in a temperature realm that has not been adequately tested to date, due to the limitations imposed by gravity.

RESEARCH APPROACH

The measurement of decay rates and correlation lengths will be achieved by using laser light scattering (time correlation spectroscopy) and turbidity measurements. Light is scattered from a near-critical fluid due to density fluctuations, which increase in scale as the critical temperature is approached, and the fluid exhibits a characteristic phenomenon known as critical opalescence. The low gravity environment of USMP-2 and the precision of both optical alignment and temperature control will allow measurements to be made much closer to the critical temperature than is obtainable on Earth.

PROGRESS DURING FY1992

The engineering development model (EDM) was completed by Ball Aerospace and delivered to the University of Maryland in January 1992. The procurement and fabrication of flight hardware were completed in FY92. All elements had been integrated except the thermostat and sample cell from the University of Maryland. Functional checkout of the system electronics showed noise levels are below requirements.

The thermostat design was modified and verified to allow for STS launch survivability. The design of optical mounts was modified and verified to resolve alignment stability problems. Groundbreaking measurements of optical heating effects were made by University of Maryland. A concept to allow for dual laser intensities at the sample cell was developed and is being implemented. A

flight-worthy sample cell was constructed. The hardware development schedule is consistent with flight on USMP-2 on February 8, 1994.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 1

— Bourkari, H, Briggs, M. E., Schaumeyer, J. N., and Gammon, R. W. "A very high-resolution thermostat for observing fluids in space." World Space Congress, Joint COSPAR/IAF Symposium on Gravity Dependent Phenomena in Fluid and Material Sciences, Washington DC, August 28 – September 5, 1992.

— Briggs, M. E., Gammon, R. W., and Shaumeyer, J. N. Measurement of the temperature coefficient of ratio transformers. Accepted for publication in *Rev. Sci. Instr.*, 1992.

— Gammon, R. W., "The ZENO experiment photon correlation light scattering from critical density xenon." World Space Congress, Joint COSPAR/IAF Symposium on Gravity Dependent Phenomena in Fluid and Material Sciences, Washington DC, August 28 – September 5, 1992.

— Gammon, R. W. 'ZENO: Photon correlation spectroscopy of critical fluctuations in microgravity on the space shuttle." Photon Correlation and Scattering: Theory and Application Conference, Boulder, CO, August 24–26, 1992.

— Schaumeyer, J. N., Briggs, M. E., and Gammon, R. W. "Statistical fitting accuracy in photon correlation spectroscopy." Photon Correlation and Scattering: Theory and Application Conference, Boulder, CO, August 24–26, 1992.

— Schaumeyer, J. N. and R. W. Gammon, R. W. "Locating the critical temperature of a pure fluid to ~ 10 μK." World Space Congress, Joint COSPAR/IAF Symposium on Gravity Dependent Phenomena in Fluid and Material Sciences, Washington DC. August 28 – September 5, 1992.

— Segre, P.N., Gammon, R.W., Sengers, J.V., and Law, B.M. Raleigh scattering in a liquid far from thermal equilibrium. *Phys. Rev. A* , *45*, 714 (1992).

— Zhang, K. C., Briggs, M. E., and Gammon, R. W. The susceptibility critical exponent for a nonaqueous ionic binary mixture near a consolute point. Accepted for publication in *J. Chem. Phys.*, 1992.

TYPE: Flight
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Heat Capacity Measurements Near the Lambda Point of Helium*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-24-04-05

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TASK OBJECTIVE/DESCRIPTION

Central to condensed-matter physics is the phenomenon of second-order phase transitions. These come about when a wide class of interactive terms is added to the simple ideal gas picture of matter. To understand condensed matter in general, it is necessary to address the phase transition issue, since phase transitions are involved in nearly all interesting effects observed. Our goal is to perform the most stringent test currently feasible of the present theory of second- order phase transitions in the asymptotic limit as the transition is approached. To do this we will measure the heat capacity of helium very close to its lambda transition at 2.177 K.

RESEARCH APPROACH

To perform the heat-capacity measurements, two main requirements must be met: first, we must have sufficient temperature resolution to establish the temperature scale, and second, we need to control the energy input to the sample to determine its heat capacity.

To these ends we have been developing a new high-resolution thermometer and an advanced, multilayer thermal control system. The thermometer makes use of superconducting technology to achieve a resolution of about 3×10^{-10} K in a 1 Hz bandwidth, and the thermal control system can achieve a power resolution approaching 10^{-12} W. These two systems give us the capability to make measurements to the limits imposed by the Space Shuttle environment. A third requirement is to achieve an operating temperature near the lambda point. TO do this we make use of the superfluid helium research facility previously flown on Spacelab-2 by JPL.

PROGRESS DURING FY1992

In February 1992 the experiment was shipped to Kennedy Space Center (KSC), where one month of preflight calibration activities were performed prior to turnover to KSC for integration with the USMP-1 carrier. Minor interface and hardware

problems were encountered and solved during the integration phase. Launch occurred on October 22. The experiment operated flawlessly throughout the mission. All systems, including high-resolution thermometers (HRT's) were found to operate perfectly after launch. Close to 100 high-resolution heat-capacity sweeps across the lambda point were performed, which promise to yield outstanding scientific results. The influence of cosmic ray events was found to be slightly worse then expected, resulting in a larger than expected thermometer noise; the impact of passing through the South Atlantic Anomaly (SAA) and the influence of acceleration noise were less than predicted. Heat- capacity data were collected from 20 mK below the transition to 1 microkelvin above. The data cellected above the transition constitute a bonus of information that was not guaranteed prior to launch. This bonus will yield important new information about the thermal conductivity in the normal phase in a region totally inaccessible from the ground.

The operation of the experiment was initially in the automatic mode, with little commanding from the ground. After the transition region was reached, and the lambda temperature was well characterized, the science team began operating the instrument almost entirely in the interactive mode, with commands being sent up from the ground to optimize data collection and initiate heat-capacity data sequences during periods of minimum disturbance. More than 5,000 commands were successfully uplinked to the experiment.

The experiment also quantified the heating effects of passing through the SAA at two different orbiter altitudes. The detailed mapping of the radiation environment of the shuttle orbit by the Lambda Point Experiment (LPE) charged particle monitors will serve as an important guide for operations planning of future planned low-temperature experiments and other investigations. Overall, the experiment has been a great success.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Chui, T. C. Comment on depression of superfluid transition temperature in 4He by a heat current. Submitted to *Physical Review Letters*, 1992.

— Chui, T. C. P., Swanson, D. R., Adriaans, M. J., Nissen, J. A., and Lipa, J. A. Temperature fluctuation in the canonical ensemble. Submitted to *Physical Review Letters*, 1992.

— Chui, T. C. P., Swanson, D. R., Adriaans, M. J., Nissen, J. A., and Lipa, J. A. Thermometry in the thermodynamic limit. *Proceedings of the 7th International Symposium on Temperature, Toronto*, 1992.

— Lipa, J. A. Advanced studies of cooperative phase transitions in microgravity. *Proceedings of COSPAR conference, Washington DC, 1992*, in press, 1992.

— Lipa, J. A., Chui, T. C. P., Nissen, J. A., and Swanson, D. R. A low temperature system for advanced thermal control. *Proceedings of 7th International Symposium on Temperature, Toronto*, 1992.

TYPE: Flight
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Critical Fluid Thermal Equilibration*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-24-05-06

PRINCIPAL INVESTIGATOR: Dr. Allen Wilkinson
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TASK OBJECTIVE/DESCRIPTION

The objective of this study is to examine the thermal relaxation and density profile versus time after a temperature perturbation of SF_6 near its liquid-vapor critical point, in a low-gravity environment. Critical-point experiments generally depend on achieving thermal equilibrium to within a specified tolerance and on knowing how phases develop or disappear. Data from this experiment will be used to determine the practical time scale needed to execute meaningful critical fluid space experiments and to characterize the location and dynamics of density or phase domains within the sample.

RESEARCH APPROACH

The SF_6 sample is to be observed using interferometry, visualization, and transmission. The scientific objectives are, first, to observe or determine the following: large-phase domain homogenization with and without stirring of the fluid; time evolution of heat and mass transfer after a temperature step is applied; phase evolution and configuration after transition from one-phase equilibrium to a two-phase state; and the effects of stirring on a two-phase low-gravity configuration; and secondly, to quantify the mass and thermal time constant of a one-phase system under logarithmic temperature steps.

PROGRESS DURING FY1992

The fiscal year began with a flurry of mission timelines and mission training. The CFTE experiment successfully flew on the European Space Agency's Critical Point Facility aboard IML-1 in January 1992. The experiment logged 60 hours of digital and videotaped interferometric fringes images, which provide a changing density map following a heat pulse.

Following the mission, activity was directed at an analysis of the information contained in these fringe patterns. A commercial software package was adapted to automate the location of fringe centers and to characterize the fringe patterns. Analytical fitting functions mapped the phase of the fringe patterns. The amplitude of the phase was tracked in time and was found to undergo exponential decay. The

time constant for this decay provides a simple parameter to describe the slowing down of heat diffusion as the critical point is approached to within a few milliKelvin. Preliminary results agree with theoretical predictions and the earlier 1-g measurements. The software techniques used were proven to be viable for this type of analysis.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Berg, R. F., Wilkinson, A., Moldover, M. R., Eicher, L., Straub, J., and Gammon, K. "Density Equilibration Near the Critical Point of SF_6 (TEQ/CPF on IML-1)." Poster at VIIIth European Symposium on Materials and Fluid Sciences in Microgravity, Bruxelles, Belgium, April 1992.

TYPE: Flight
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Measurement of Liquid-Liquid Interfacial Tension*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-26-04-02

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TASK OBJECTIVE/DESCRIPTION

The objective of this task is to perform measurements of small liquid-liquid interfacial tension in microgravity. This test will establish the feasibility of using the same technique at high temperatures to determine the interfacial tension between to phases of liquid glass and thereby assess the role of gravity in phase separation kinetics. Using two slightly miscible organic fluids, the Drop Physics Module creates a drop of one fluid inside a drop of the other. This compound drop is rotated and photographed from several angles. From the shapes of the two interfaces at a given rotation rate the interfacial tension will be determined.

RESEARCH APPROACH

To prepare for the flight, appropriate sample-fluid pairs were identified and their relevant physical properties measured; existing theory was used to select the optimal volumes and rotation rates to provide the most sensitive test matrix for determining the interfacial tension.

PROGRESS DURING FY1992

During the USML-1 mission, the astronauts and DPM were unable to form the desired compound drops. Images of drops containing both fluids are being studied. Discolored fluid returned from the mission is being analyzed.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Podlesny, J., Neilson, G. F., and Weinberg, M. C. Sample preparation methods for SAXS study of phase separation in lead rotate glasses. *Materials Letter 13,* 267 (1992).

— Yasumori, A., Neilson, G. F., and Weinberg, M. C. Measurement of surface tension of organic liquid pairs. *J. Colloid Interface Sci.,* accepted 1992.

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *In-Situ Monitoring of Crystal Growth Using MEPHISTO*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-25-05-04

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TASK OBJECTIVE/DESCRIPTION

The aim of this collaborative study is to investigate the solidification behavior and the stability of the solid/liquid interface during growth of pure bismuth (a facet-forming material) and bismuth with a small amount of tin.

RESEARCH APPROACH

Experiments are defined to make use of the second flight of MEPHISTO on USMP-2. The first flight (USMP-1, September 1992) was for the purpose of studying the morphological stability in tin alloyed with bismuth, conducted by Dr. Favier of the Centre d'Etudes Nucleaires.

PROGRESS DURING FY1992

Progress has been made in preparation of crystals for flight specimens and for ground testing in the MEPHISTO at Toulouse, France, and for testing at the University of Florida.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Effects on Nucleation by Containerless Processing*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-25-08-06

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TASK OBJECTIVE/DESCRIPTION

There is both a scientific and practical objective of the work. The primary scientific objective is to further the understanding of nucleation of solids from their melts. Within the envelope is a concern for the role of melt agitation on nucleation. The practical objective is to determine, in qualitative terms, the necessity for containerless processing in low Earth orbit, with regard to nucleation studies.

RESEARCH APPROACH

All possible ground-based methods are being investigated for applicability to containerless processing of bulk samples of pure metals. Comparisons of the data from the ground-based techniques give evidence as to the nature of the nucleation of the solid from the liquid. Different processing methods have different environments and other factors that may affect the amount of undercooling in bulk samples. Since nucleation is a statistical process, approximately one hundred undercooling measurements are recorded for each type of sample. This number of measurements allows for statistical assumptions to be made, thereby easing the interpretation of results. In addition, considerable effort on contactless temperature-measurement techniques is being made. Increasing the precision of temperature measurement is an important part of the experiments because of its dramatic effect on the results.

PROGRESS DURING FY1992

Nucleation frequency experiments on zirconium were conducted using the Marshall Space Flight Center Drop Tube Facility and the electromagnetic levitation apparatus at Vanderbilt University. Temperature measurement at both locations was done by optical pyrometry. Experiments were done on 99.5% pure stock and 99.95% pure stock.

Over the entire sample set, maximum undercoolings ranged from 13% to 15% of the equilibrium freezing temperature, but higher-purity samples tended to produce higher undercoolings. Also, a fundamental difference in the distribution of

undercoolings was seen in the different environments. A low undercooling tail was present in the levitator undercooling distribution, whereas a similar tail was not observed in the drop tube. In both cases, calculations based on the Skripov approach to the analysis of nucleation experiments yielded values in the heterogeneous regime for the exponential and preexponential factors in the nucleation rate equation.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Hofmeister, W. H., Morton, C. W., Bayuzick, R. J., Robinson, M. B., and Rhetz, T. J. "Analysis of the constraints in statistical analysis of nucleation data in ground-based experiments." TMS Annual Meeting, San Diego, CA, September 1992.

— Morton, C. W., Hofmeister, W. H., Bayuzick, R. J., and Robinson, M. B. "Statistical analysis of nucleation temperatures from two containerless processing methods." TMS Annual Meeting, San Diego, CA, March 1992.

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Alloy Undercooling Experiments in Microgravity Environment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-25-05-03

PRINCIPAL INVESTIGATOR: Prof. Merton C. Flemings
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TASK OBJECTIVE/DESCRIPTION

To evaluate/develop techniques to measure the effects of undercooling and microgravity processing on phase formation, solidification velocity, and microstructure development in selected alloys.

RESEARCH APPROACH

Research is designed to: (a) produce high-purity alloy specimens and process them, using electromagnetic levitation with simultaneous high-speed temperature measurement; (b) solidify specimens after high undercooling by flowing gas or quenching in liquid metal; (c) perform detailed analyses of alloy microstructures produced using a variety of optical, electron, and X-ray analytical techniques; model solidification behavior during the entire solidification process from the undercooled liquid, including recalescence, dendrite growth, coarsening, and grain formation; and (e) perform similar experiments in microgravity and compare results with those of ground-based research.

PROGRESS DURING FY1992

Work during the past year has focused on obtaining baseline data and a fundamental understanding of the solidification of undercooled alloys, in preparation for the flight experiments. The ground-based work has included a detailed investigation of the relationships between processing conditions, undercooling, dendrite growth, and microstructure development in the Ni-Sn and Fe-Ni alloys which are planned for the flight experiment. In addition to high-speed pyrometric temperature measurements, extensive microstructural studies have been performed using a number of different analytical techniques. The microstructure investigation includes work on microsegregation, dendrite branching grain structure, morphology transitions, texture analysis, and coarsening. Modeling and calculations of heat flow and solute segregation during recalescence

and throughout the entire solidification process have been carried out for the processing conditions used in the experiments.

In preparation for the flight experiments, we have revised science definition statements and flight experiment protocols, have reviewed TEMPUS hardware plans and designs, and have participated in Investigator Working Group (IWG) meetings and crew training sessions.

Specimens for calibration experiments in the ground support facility in Cologne, Germany were prepared and delivered. Flight specimens have been prepared and are nearly ready for delivery.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Zhao, Q., Brody, H. D., Piccone, T. J., and Fleming, M. C. "Dendrite growth of highly undercooled Ni-Sn alloys." 1992 TMS annual meeting, San Diego, CA, March 3, 1992.

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Gravitational Role in Liquid-Phase Sintering*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-25-05-05

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TASK OBJECTIVE/DESCRIPTION

The purpose of this research is to establish how gravity influences the macro-and microstructural development of tungsten heavy allows during liquid-phase sintering (LPS).

RESEARCH APPROACH

Experiments in space will determine grain growth-kinetics without settling and gravity-induced liquid convection. The investigation is in the definition phase, where science requirements will be established. The investigation may then be confirmed for the execution phase, if it is approved for flight. If flown, the experiment will be conducted in the Japanese-developed large isothermal furnace (LIF) on the IML-2 mission.

PROGRESS DURING FY1992

The principal investigator, Prof. German, completed a successful Flight Science Readiness Review (FSRR) in June 1992. All of the samples sintered in the large isothermal furnace (LIF) engineering model facility at the IHI Mizuho plant in Tokyo, Japan, have now been returned to Pennsylvania State University. During this reporting interval the analyses of the 1-minute and the 120-minute samples were finished.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Isothermal Dendritic Growth Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-25-05-01

PRINCIPAL INVESTIGATOR: Dr. Martin E. Glicksman
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TASK OBJECTIVE/DESCRIPTION

The Isothermal Dendritic Growth Experiment (IDGE), to be performed on three of the United States Microgravity Payload (USMP) flights, starting with USMP-2, is designed to provide microgravity data on dendritic growth for a critical test of theory.

Dendrite crystallization is common in most industrial casting and welding processes, and it remains a subject of interest to both scientists and engineers attempting to understand the factors that control dendritic patterns and microstructures and nonlinear dynamic patter formation in general. Current theories of dendritic pattern formation are based primarily on diffusive transport, with convection either ignored altogether or added as a separate phenomenon.

In actuality, the simultaneous presence of convection and diffusion during dendritic growth in the presence of Earth's acceleration field results in coupled transport that in turn, alters the dendritic "operating state," which is often expressed as the speed and size scale of the crystals for a given supercooling or thermal driving force. The ability to perform a critical test of dendritic growth theory depends on the availability of a suitable experimental system that provides precise, quantitative, thermodynamic driving forces acting on a well-characterized material. IDGE is designed to meet these specifications.

RESEARCH APPROACH

The first IDGE flights, scheduled for the USMP-2 mission in February 1994, will measure dendritic growth events in succinonitrile (SCN; $CN\text{-}(CH_2)_2\text{-}NC$), a transparent, body-center-cubic plastic crystal that freezes with characteristics similar to cubic metals, and therefore acts as an analog for metal solidification. Furthermore, SCN's thermophysical properties are well characterized; it is transparent to visible light, has a convenient (for experimentation purposes) melting temperature, and therefore serves as an excellent test substance for this investigation.

Ground-based measurements have clearly delineated the influences of gravity on the dendritic growth process. Specifically, gravity-driven convection (natural or buoyancy-driven convection) starts to affect the growth rate and crystal morphology of SCN dendrities when the supercooling is less then about 1.2 K. At large supercoolings (> > 1 K) gravity plays a minor role, because convection provides weak transport relative to thermal diffusion. Buoyancy-driven convection arises spontaneously from the interaction of the gravitational body force with the microscopic density gradients produced in the fluid phase by the thermal transport field responsible for the flow of latent heat from the solid to the supercooled melt. Then buoyancy-driven convection becomes an increasing and then an overwhelming kinetic factor as the supercooling decreases. Unfortunately, it is only at small supercoolings, where gravity effects dominate, that the kinetic conditions are suitable for checking dendritic growth theories.

Thus, the first IDGE flight will perform photographic observations at a variety of supercoolings in the 0.1 K – 1.0 K range. A novel growth chamber, millikelvin thermostat, and optical system have been developed to accomplish this task, for operation in orbital microgravity, under semi-autonomous conditions. In addition, IDGE science and engineering teams have developed a photographic analysis system and automated techniques to extract data from the IDGE photographs.

The IDGE growth chamber permits a single sample of SCN (greater than 5-9's purity) to be repeatedly melted, supercooled, nucleated, and photographed on orbit. Dendritic growth velocity and tip radii measurements can be derived from optical measurements for each of the selected supercoolings. IDGE provides two independent optical axes for stereographic correction. Up to 250 35 mm photographs can be taken, which allows up to 20 independent dendritic growth sequences at the preselected supercoolings, where 10 photographs (one for each mm of growth) record each supercooling and each optical axis.

On-board accelerometry—derived from the SAMS—temperature measurement and control, and data for other relevant experimental conditions, including slow-scan video down-link of the dendritic growth events, are all available during flight in near real time to the payload operations control center from the IDGE. Up-linking of a restricted set of commands for the adjustment of the experimental protocols, including experiment interruption, repeated runs, shift of supercooling, etc., are also communication features of the IDGE.

Future integrated ground-based test using the flight hardware will provide both pre- and post-flight ground-based data sets. Any difference between the microgravity and terrestrial data sets, using the same growth chamber, material and ancillary apparatus, will demonstrate conclusively the effects of microgravity on dendritic growth and provide a critical test of theory.

PROGRESS DURING FY1992

In FY 1992 the project has achieved considerable success. The Principal Investigator, his science and engineering team, and the NASA LeRC IDGE engineering team have spent considerable efforts on the continued integrated tests of the IDGE prototype engineering hardware and the subsequent analysis and data reduction. This work was incorporated into the final design and manufacture of the flight hardware and analysis tools.

The results of this work, both at Rensselaer and LeRC, have contributed to the latest Science Verification Review (SVR) results. In these tests, the dendritic velocity data have little scatter, and are consistent with the historical (conventional laboratory) data set.

The radii data exhibit more scatter than do the velocity data. The differences between the IDGE and historical data are due, primarily, to the differing chamber sizes supporting different states of natural convection. At present, for supercoolings equal to or greater than 0.77 K. we are unable to analyze shadowgraphic photographs for dendritic radii and maintain an uncertainty of less than 5%, which is our goal. However, the lack of determinacy in the radii data at the larger supercoolings is not an insurmountable problem, because we can use the velocity data to correlate the historical, the IDGE ground-based, and the IDGE space-flight data sets. At the lower supercoolings, both the radii and velocity data are easily measured, and the differences between space-flight and ground-based data should be clearly distinguishable.

These improved SVR results were achieved in many ways. Extensive numerical modeling showed that the differences between the Science Verification Review (SVR) data and the historical data could not be explained by gaussian scatter in the photographic edge function. Nor could the gaussian scatter explain the radii in the SVR data sets. These tests also indicated how the gaussian scatter in the edge function could contribute to the radii scatter in the data, and how to minimize this by analytical methods. Curve-fitting tests yield information on how to compare differing data sets.

Detailed examination of the photographic negative subsequently revealed three sources of scatter: (a) some dendrities grow so close to neighboring dendrities that they are no longer isothermal; (b) some dendrities grow so that a crystallographic [110] profile is presented to the optic system, rather that a [100] profile, and whereas the [110] profile has a parabolic shape for a much smaller distance from the dendrite tip, the tips can appear to be too small; (c) some dendrites have not achieved steady-state growth by the time they leave the field of view. The problems associated with nonisothermal and non-steady-state dendrite tips have hardware fixes that will be described later. For the situation of the [110] profiles, they will simply have to be recognized and separated from the rest of the data set. We also discovered that the background illumination, attributed to the flash unit in the

engineering unit, provided a nonuniform light intensity that was detrimental to the photographic analysis. This too has been fixed through the modification of the optic system on the flight unit.

During FY 1992 we have taken the results for the SVR tests on the engineering hardware, incorporated improvements to the flight hardware design, constructed MOD III or flight quality growth chambers, filled one flight quality chamber with 5-9's pure SCN, completely tested and retested that chamber, and delivered it to LeRC. We also filled and partially tested a second flight quality chamber, and are waiting for the delivery of an improved and sturdier thermoelectric cooler unit to use in completing the assembly of this second chamber.

The most critical and obvious hardware design change has been to the stinger. It has been moved higher into the chamber so that a dendrite emerging from the tip has the entire field of view of the photographic frame in which to grow. In addition the stinger has been notched, much like the tip of a fountain pen, so as to isolate the dendrite tips better and increase the probability of isothermal growth conditions. Tests at Rensselaer show that this latter change was successful.

Many less obvious changes have also been made to the chambers and in the way we handle the manufacturing process. The windows have been polished; the thermistors have been aged to reduce their drift. Our laboratories at Rensselaer have been changed so as to separate and isolate the laboratory-based growth-chamber work from the data analysis operations, thereby reducing the possibility of contaminating the growth chambers. The piece parts to the chambers have been, at several intermediate stages, cleaned and bagged in a microelectronic clean room facility at the Center for Industrial Innovation (CII) here at Rensselaer. Finally, all parts of the cleaning, filling, and testing procedures were fully documented and followed to insure rigorous reliability and quality assurance.

At the end of FY 1992 we had fully implemented a computer aided dendrite analysis program (CADAP), version 1.2, running on a 486-based computer. This program evolved from the work at both Rensselaer and LeRC over the last several years. CADAP, however, is not stand-alone, but is used best in conjunction with the precision optical state (ROI) that we have used the last few years. The ROI now has a black-and-white camera with variable gamma function and on/off automatic gain control. Furthermore, CADAP is only used for measuring radii. Velocities, magnification of the flight optic system, dendritic growth angle for the sterographic correction, transmission data for the image processing, etc. are measured on the ROI or other instruments, and the results are input to CADAP if required. We intend to test and complete the development of CADAP and ancillary apparatus and methods early in FY 1993, with the arrival of the first few integrated mission simulations using the flight chamber with the flight hardware.

Finally, we have continued to make progress for the second and third IDGE flights. We have filled and begun testing a pivalic acid (PVA) engineering growth chamber, and are continuing to seek improvements in the day-to-day operation of our laboratories. Our new vacuum distillation system has produced enough SCN for the current and future flights, and we are beginning a production run to produce high-purity PVA.

GRADUATE STUDENTS: 5   **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Glicksman, M., Koss, M., Hahn, R., Koo, K., Rojas, A. and Wansa, E. The isothermal dendritic growth experiment: A USMP-2 space flight experiment. Preprinted AIAA 92-0350 of the *30th Aerospace Science Meeting & Exhibit*, Reno, NV (1992).

— Glicksman, M., Koss, M., R. Hahn, R., Rojas, A., Karthikeyan, M., and Winsa, E. The isothermal dendritic growth experiment: scientific status of a USMP-2 space flight experiment. Advances in Space Research, *Proceedings of the COSPAR Symposium on Microgravity Research: Materials and Fluid Sciences*. World Space Congress. In preparation 1992.

— Glicksman, M., Koss, M. K., Koo, K., Hahn, R., Rojas, A., and Winsa, E. Isothermal dendritic growth in microgravity. *Proceedings of the 4th International Conference on Experimental Methods for Microgravity Materials Science Research*, Robert A. Schiffman, ed., p. 147, Warrendale, PA: The Minerals, Metals & Materials Society, 1992.

— Koo, K. "Dendritic growth in microgravity." Transport and Stability Phenomena in Crystal Growth/Session I, AIChE Los Angeles, 1992.

— Koss, M. "The isothermal dendritic growth: A NASA microgravity experiment." Department of Physics and Astronomy Seminar, Vassar Collage, Poughkeepsie, NY, 1992.

— Koss, M., "Isothermal dendritic growth experiment: Scientific status of a USMP-2 space Flight Experiment." COSPAR/IAF, World Space Congress, Washington DC, 1992.

— Koss, M., "The isothermal dendritic growth experiment: A status report." Materials Engineering Department Seminar, Rensselaer Polytechnic Institute, Troy, NY, 1992.

— Winsa, E. "Isothermal dendritic growth experiment flight unit tests." COSPAR/IAF, World Space Congress, Washington DC, 1992.

— Winsa, E., Levinson, L., Glicksman, M., Hahn, R., Koss, M., Robertson, J., and Abramczyk, R. Isothermal dendritic growth experiment flight unit test. *Advances in Space Research. Proceedings of the COSPAR Symposium on Microgravity Research: Materials and Fluid Science.* World Space Congress. In preparation, 1992.

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Thermophysical Properties of Metallic Glasses and Undercooled Alloys*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-25-08-07

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TASK OBJECTIVE/DESCRIPTION

The objectives are to (a) study physical properties of undercooled metallic alloy melts that relate to glass formation,. and (b) develop calorimetric methods to investigate the specific heat and thermal conductivity of alloy melts, both in the equilibrium and undercooled state.

RESEARCH APPROACH

Steps will be taken to :

1. Carry out ground-base measurements of the specific heat of glass-forming liquid alloys using a differential scanning calorimeter and a drop calorimeter;

2. Develop a noncontract AC calorimetery method for high-melting-point transition metal liquid alloys which can be implemented using the TEMPUS facility on the IML-2 mission;

3. Implement the AC methods using TEMPUS hardward and software. (Samples chosedn for study are Zr_3Ni and $Nb_{40}Ni_{60}$ liquid alloys);

4. Provide samples of the two alloys to Dr. Shankar Krishnan at Intersonics Corporation in Chicago for spectral emissivity measurements at 633 mm; use this date to calibrate temperature measurement on TEMPUS;

5. Develop a ground-base blackbody balometer for measureing the total hemisphereical emissivity of levitated liquid samples that will be used to calibrate the heat flow in the flight experiments;

6. Carry out measurements of total hemispherical emissivity of the samples for the flight experiments;

7. Develop a complete set of software input parameters for carrying out the AC, specific heat measurement using the TEMPUS facility;

8. Carry out specific heat measurements on liquid Zr-Ni and Nb-Ni alloys both above and below the thermodynamic melting point of the alloys during the IML-2 flight of TEMPUS, use this data to calculate the entropy and free-energy functions for the equilibrium and undercooled liquids and determine the Kauzmann isentropic temperature of the undercooled liquids, comparing it to the observed glass transition temperature of the alloys; and

9. Analyze data obtained during the flight experiments, assess the results in terms of classical nucleation theroy, and relate the results to the glass-forming ability of the alloys.

PROGRESS DURING FY1992

During FY1992, we completed the design of the ground-based blackbody balometer for measuring the total hemispherical emissivity of liquid samples. We are currently constructing the device in collaboration with the group of E. Trinh and K. Ohsaka at JPL, and will mount the balometer on a levitation system at JPL.

We have also carried out ground-based specific heat measurements on Ti–Cr alloys, using both a drop calorimeter and a differential scanning calorimeter, and analyzed these results [J.C. Holzer et. al., Appl. Phys. Lett., 60, 1079 (1992)]. Workin with H. J. Fecht and R. Wunderlich, we are carrying out ground-based tests of the AC calorimetry method using the TEMPUS demonstrator module at DLR in Cologne, Germany; the AC method has been successfully demonstrated in the TEMPUS laboratory prototype by R. Wunderlich.

Measurements of the specific heat of a solid Nb sphere were carried out successfully (liquids cannot be levitated in the TEMPUS demonstrator). Samples of Zr–Ni and Nb–Ni have been sent to DLR for evaluation of evaporation rates, etc. Samples also have been sent to S. Krishnan for spectral emissivity measurements at 633 nm.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Fecht, H. J. Aspects of metastable phase formation in undercooled liquid leud alloys. *Zeit for Metallkunde*, 82, 186 (1991).
— Fecht, H. J. Free energy; function of undercooled glass forming liquids. Accepted for publication in *Mat Sci, & Eng., A133*, 443 (1991).
— Fecht, H. J. Phase selection during crystallization of undercooled liquid eutectic alloys, *Acta Metturgica*, 39, 1003 (1991).
— Holzer, J. C., Ohsaka, K., Trinh, E. H., and Johnson, W. L. Gibbs free energy difference between the undercooled liquid and the β Phase of a Ti–Cr alloy. *Appl. Phys. Lett.*, 60, 1079 (1992).
— Ohsaka, K., Holzer, J. C., Trinh, E. H., and Johnson, W. L. Specific heat measurement of undercooled liquids. *Proc. TMS Symp.*, TMS–AIME March meeting, in press (1992).

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Casting and Solidification Technology*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-25-08-05

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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to: (a) perform a detailed characterization of the effects of convection on growth parameters for unidirectional dendritic solidification; and (b) measure solutal and thermal fields of dendritically solidifying model material using the fluid experiments system (FES) holographic recording, and compare the results to mathematically derived models and to Earth-based results.

RESEARCH APPROACH

A threefold approach was adopted for the successful completion of this project:

1. Performance of extensive ground-based directional solidification experiments, during which a variety of optical techniques are used to record and analyze the thermal and solutal fields;

2. Development of two computational models, the fluids thermal model (FTM) and the linear stability model (LSM), for predictions of the dendritic solidification process and the onset and character of the fluid flow; and

3. Development of a matrix of eleven microgravity experiments conducted in the FES, from which thermal and solutal fields will be obtained for comparison with ground-based and computation model predictions.

PROGRESS DURING FY1992

The CAST experiment flew on IML-1 during January 1992. Eleven experiments were completed, nine of which had acceptable holographic data. Growth front height as a function of time was obtained for eight of the runs from the reconstructed ground-based and flight holograms. Growth rates were determined from linear curve fits, starting with the time at which the holographic data indicated the the dendritic front was uniformly distributed across the curvette. The ground-based dendritic growth rates are lower than the flight growth rates for seven

of the eight runs analyzed and are approximately one-half of the flight rate for six of the runs. The decrease in growth rate at 1-g can be attributed to the gravitational influence on fluid flow and the resultant change in concentration of the liquid into which the dendrites are growing.

This effect is also seen in another significant difference between the ground-based and flight growth structure. The mushy zone is not transparent in the ground-based experiment whereas it is transparent in flight experiment, and individual dendrites can be distinguished. This demonstrates the role that the buoyancy mass transport mechanism plays in influencing the concentration of the interdendritic liquid within the mushy zone and the volume fraction of solid formed. As the extent of convection increases, the interdendritic fluid concentration increases, owing to the movement of higher solvent concentration fluid into the mushy zone. The higher solvent concentration adjacent to the dendrites produces more solidification and a higher-volume fraction of solid.

FTM predictions for 10^0 and 10^{-5} g_e were validated using the flight and ground experiment results for a selected run. Dendritic growth front predictions for the intermediate gravity levels show that as the gravity forces decrease, the growth rates increase until approximately 10^{-4} g_e, at which they level off. The maximum flow velocities decrease with gravity level, approaching the zero-gravity value at 10^{-3} g_e. The flow remaining below 10^{-3} g_e, can therefore be attributed to mass flow effects other than those related to buoyancy.

These results indicate that buoyancy-driven flow can be minimized in microgravity, enabling analysis of the two remaining mass flow mechanisms, shrinkage and solutal diffusion, and their influence on the dendritic growth front. This is currently being done using the computational models and thermal and solutal profiles which have been obtained from the flight experiments holograms.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 3

PUBLICATIONS/PRESENTATIONS

— Hopkins, J. A., McCay, T. D., and McCay, M. H. "The effects of shrinkage flow and gravity level on the onset of convection during vertical directional dendritic solidification of NH_4Cl-H_2O." Presented at the 31st Aerospace Sciences Meeting & Exhibits (AIAA), paper #AIAA93-0261, Reno, NV, 1992.

— Lowry, S. A., McCay, T. D., and McCay, M. H. "An ad hoc non-equilibrium numerical model of the solidification of the binary metal model NH_4Cl-H_2O." Presented at The American Society of Mechanical Engineers, Winter Annual Meeting, Anaheim, CA, 1992.

— Lowry, S. A., McCay, T. D., and McCay, M. H. An ad hoc non-equilibrium numerical model of the solidification of the binary metal model NH_4Cl-H_2O. *Micro/macro scale phenomena in solidification, ASME 1992.* C. Beckermann, L. A. Bertranm, S. J. Pien and R. E. Smelser, eds., HTD-vol. 218/AMD-vol. 139, 1992.

— McCay, T. D., and McCay, M. H. Measured and predicted effects of gravity level on directional dendritic solidification of NH_4Cl-H_2O. Accepted for publication in *International Journal for Microgravity Research and Applications*, 1992.

— McCay, M. H., and McCay, T. D. The measurement of transient dendrite tip interface supersaturation in NH_4Cl-H_2O using optical techniques. Accepted for publication in *Journal of Crystal Growth*, 1992.

— McCay, M. H., and McCay, T. D. "An optical study of grain formation: CAST International microgravity laboratory I." Presented at the 8th European Symposium on Materials and Fluids Science in Microgravity.

— McCay, T. D., McCay, M. H., and Hopkins, J. A. Heat and mass transfer effects on dendrite growth during vertical directional solidification of NH_4CL-H_2O. Accepted for publication in *Journal of Materials Processing and Manufacturing Science*, 1992.

TYPE: Flight
DISCIPLINE: Metals and Alloys
PROJECT TITLE: ***Measurement of Viscosity and Surface Tension of Undercooled Melts***
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-25-08-08

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TASK OBJECTIVE/DESCRIPTION

The objective of this investigation is to utilize the electromagnetic levitation unit, TEMPUS, on IML-2 to measure the viscosity and surface tension of undercooled metallic melts. To date, little study has been made of the erhermophysical properties of undercooled melts, and a controversy exists over whether the temperature dependence of the viscosity obeys an Arrhenium-type or a power-law relationship. In this investigation, a "squeezing" force will be applied to a suitably positioned sample to induce oscillations. The rate of decay of the amplitude of these oscillations will be observed in order to measure the viscosity at a number of temperatures in the undercooled regime, while the frequencies of the oscillation modes will be used to deduce the surface tension at these temperatures.

RESEARCH APPROACH

Our effort consists largely of a comprehensive program of mathematical modeling designed to give a detailed understanding of what can be expected from the flight experiment. To date, the main thrust of the modeling work has been to develop the methodology and to perform calculations predicting the behavior of levitation-melted/electromagnetically-positioned metallic droplets under both earthbound and microgravity conditions.

The main purpose of the work was to be able to predict the electromagnetic forces and heating rates, electromagnetically driven velocity fields within the sample, the transient behavior of the system, and the deformation of the sample. The accuracy of the computational models have been checked by comparison with available analytical results and the results of ground-based experiments.

PROGRESS DURING FY1992

We have improved our mathematical model of the free surface shape of an electromagnetically shaped molten metal droplet by including the effects of fluid flow; this had previously been neglected. We accomplished this using the

electromagnetics code we developed with the FIDAP computational fluids package, which has the ability to include electromagnetic body forces and surface shapes and affords excellent graphics. Using our FIDAP-based model, we have also achieved preliminary success in what was thought to be one of the most difficult aspects of the modeling effort: simulation of the oscillations that the electromagnetically-positioned and perturbed samples undergo.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

— Schwartz, E., Szekely, J., Ilegbusi, O. J., Zong, J-H., and Egry, I, "The Computation of the electromagnetic force fields and transport phenomena in levitated metallic droplets in the microgravity environment." *Proc. of Symposium on Magnetohydrodynamics in Process Metallurgy,* p 81, TMS 1992.

— Zong, J-H., Li, B., and Szekely, J. "The electrodynamic and hydrodynamic phenomena in magnetically-levitated molten droplets I." Steady state behavior. Accepted for*Acta Astronautica,* 1992.

— Zong, J-H., Li, B., and Szekely, J. "The electrodynamic and hydrodynamic phenomena in magnetically-levitated molten droplets II." Transient behavior and heat transfer considerations. Accepted for *Acta Astronautica,* 1992.

— Zong, J-H., Szekely, J., and Lohofer, G. "Calculations and experiments concerning the lifting force and the power absorption in the TEMPUS EML. Accepted for*Acta Astronautica,* 1992.

— Zong, J-H., Szekely, J., and Schwartz, E. "An improved computational technique for calculating electromagnetic forces and power absorptions generated in spherical and deformed body in levitation melting devices." *IEEE Transactions on Magnetics, 28,* 1833 (1992).

TYPE: Flight
DISCIPLINE: Protein Crystal Growth
PROJECT TITLE: *Protein Crystal Growth in a Microgravity Environment*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-23-08-02

PRINCIPAL INVESTIGATOR: Dr. Charles E. Bugg
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are: a) to produce larger, high quality protein crystals in microgravity; and b) to understand the dynamics and processes of protein crystal growth. The research will utilize the protein crystal growth (PCG) vapor diffusion apparatus (VDA) flight hardware that will be capable of determining protein molecular structures for applications in medicine, drug design, agriculture, and the biological sciences.

The flight investigations utilized proteins from a number of co-investigators at universities and pharmaceutical companies. These proteins selections were based on a number of criteria, including: (a) availability of extensive ground-based, 1-g visual and x-ray data; (b) crystal growth time; (c) crystal stability; and (d) inherent problems with crystal quality that might benefit from exposure to a microgravity environment (e.g., crystal size, internal crystal quality, crystal sedimentation, etc.).

RESEARCH APPROACH

Proteins were selected by a committee composed of co-investigators from academia, industry, and NASA's Marshall Space Flight Center (MSFC). Several months of ground-based experiments were performed in flight-like hardware by each investigator whose protein had been selected for upcoming Space Shuttle flights. Crystallization conditions were optimized in this hardware in an effort to maximize the success rate during the flight experiment.

During the 1992 time frame, protein crystal growth experiments were flown on IML-1, SL-J, and USML-1. For the first United States Microgravity Laboratory mission, new hardware was developed that utilized the Glovebox flown in the Spacelab module. The Glovebox hardware allowed, for the first time, optimization of protein crystal growth experiments and provided better mixing procedures for viscous protein/precipitant solutions.

In addition, a micromanipulator system was developed to allow seeding experiments and crystal mounting procedures to be undertaken. A special adapter

for the Glovebox video system, as well as a binocular microscope, allow crystals observed by the crew to be downlinked for analysis by co-investigators in the POCC.

PROGRESS DURING FY1992

Through the series of missions flown in 1992, and in conjunction with the co-investigator group, it has been demonstrated that the microgravity environment provided by the Space Shuttle can enhance the size and/or quality of protein crystals in a significant fashion. Resolution enhancements as great as 0.6 Å have been observed, and, in several instances, crystal volume increased twofold. In addition, it was clearly demonstrated on USML-1 that crystal optimization can increase the success of these experiments and that crystal mounting via a micromanipulator is straight forward, thereby providing a method to collect data on crystals once an X-ray facility is available on Space Station Freedom.

Ground-based work carried out at UAB, MSFC, and MSU has continued to provide a better understanding of the fundamental mechanisms involved during crystal nucleation and subsequent growth phases. Using both a hanging drop (vapor diffusion) configuration or batch/temperature-induced crystallization system, it has been demonstrated that static light scattering can be an effective tool to detect the onset of crystal nucleation so that the growth phase can be dynamically controlled.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— DeLucas, L. J., "Protein crystal growth results from the United States Microgravity Laboratory - 1 Mission." Presented at the Second International Workshop on Crystal Growth of Organic Materials (CGOM2), Glasgow, Scotland, September 7-11, 1992.

— DeLucas, L.J., Bugg, C. E., et. al. Recent results and new hardware developments for protein crystal growth in microgravity. Submitted to *Journal. of Crystal Growth*, 1992.

— DeLucas, L. J., Moore, K. M., Narayana, S. V. L., Bray, T. L., Rosenblum, W. M., Einspahr, H. M., Clancy, L. L., Rao, G. S. J., Harris, B. G., Munson, S. H., Finzel, B. C., and Bugg, C. E. Protein crystal growth experiments and results from the United States Microgravity Laboratory - 1 Mission. Submitted to *Journal. of Crystal Growth,*. 1992.

TYPE: Flight
DISCIPLINE: Protein Crystal Growth
PROJECT TITLE: *CRYOSTAT*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-23-08-07

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TASK OBJECTIVE/DESCRIPTION

The preflight research goal of the IML-1 experiment was to purify and characterize two macromolecular samples, canavalin and satellite tobacco mosaic virus (STMV), and to develop procedures whereby the samples could be reproducibly crystallized using the liquid-liquid diffusion method.

The goal of the flight experiment was to crystallize these samples in a form suitable for subsequent optical examination and X-ray diffraction analysis and to compare results with parallel experiments conducted in a ground laboratory. The instrument designated for the flight experiment was CRYOSTAT, designed by DARA scientists and fabricated by Keyser-Threade of Munich, Germany. Co-Investigators on the experiment from Europe were Professor Walter Littke of Freiburg and Professor Gottfried Wagner of Geissen.

RESEARCH APPROACH

The approach employed to bring about crystallization of canavalin and STMV in microgravity was liquid-liquid diffusion (free interface diffusion) using protein and precipitant volumes of 0.7 ml with a spacer or buffer 2 mm. thick initially inserted between the interdiffusing samples. Two sample carriers were employed in the experiment that was carried itself in the spacelab module. One sample carrier (containing 7 samples) was maintained throughout flight at 23 °C while the second container with the same number of samples, was thermally ramped over the 7-day mission from 0 °C to 23 °C. Three canavalin samples were flown and four STMV samples. The remaining sample cells were used by the European co-investigators.

In parallel with the CRYOSTAT experiment, identical protein and virus samples were also crystallized using vapor diffusion in the VDA (designated code PCG). Two R/IM modules were flown carrying VDA samples maintained in one case at 4 °C and at 23 °C in the other.

Six samples of canavalin and six of STMV were investigated in each of the two R/IMs. The crystals grown by vapor diffusion were compared with both ground-grown samples and with those grown in CRYOSTAT by liquid-liquid diffusion.

PROGRESS DURING FY1992

The flight of IML-1 was carried out at the end of January 1992 in the spacelab module on orbiter Columbia and the samples retrieved immediately upon landing. Samples were returned to the laboratory at UCR and analyzed by light microscopy and X-ray diffraction. Crystals grown in CRYOSTAT, in the VDA, and in ground controls were compared.

Crystals were grown in virtually every trial, but the characteristics of the crystals were highly dependent on the crystallization technique employed and the temperature experience of the sample. In general, very good results, based on visual inspection of the crystals, were obtained in both PCG and CRYOSTAT. Unusually impressive results were, however, achieved for STMV in the CRYOSTAT instrument. STMV crystals grown in microgravity by liquid-liquid diffusion were more than tenfold greater in total volume than any STMV crystals previously grown in the laboratory.

X-ray diffraction data collected from eight STMV crystals grown in CRYOSTAT demonstrated a substantial improvement in diffraction quality over the entire resolution range when compared to data from crystals grown on earth. In addition, the extent of the diffraction pattern for the STMV crystals grown in space extended to 1.8 Å resolution while the best crystals that were ever grown under conditions of earth's gravity produced data limited to 2.3 Å resolution.

Other observations suggest that the growth of macromolecular crystals is indeed influenced by the presence or absence of gravity. These observations further suggest, consistent with earlier results, that the elimination of gravity provides a more favorable environment for such processes.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Day, J., and McPherson, A. Macromolecular crystal growth experiments on International Microgravity Laboratory-1. *Protein Science* 1, 1254–1268, (1992).

— McPherson, A. "Effects of a microgravity environment on the crystallization of biological macromolecules." *Proceedings VIIIth European Symposium on Materials and Fluid Sciences in Microgravity*, Brussels, Belgium, 12–16 April, Vol. II, 619–626 (1992).

TYPE: Ground
DISCIPLINE: Biotechnology
PROJECT TITLE: ***Biosynthesis of Cellulose under Microgravity Conditions***
RESPONSIBLE CENTER: JSC **PROJECT IDENTIFICATION:** 674-23-01-04

PRINCIPAL INVESTIGATOR: Prof. R. Malcolm Brown
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TASK OBJECTIVE/DESCRIPTION

The object of this grant is to determine the effects of microgravity on cellulose biosynthesis.

RESEARCH APPROACH

Investigators developed methodologies to observe and measure active cellulose synthesis. The three-dimensional arrangement of cellulose linkages was studied under 2-g, 1-g, and low-g simulations in a KC-135. Cellulose, which is typically ribbon shaped, began to splay under microgravity conditions simulated in a KC-135. Data suggests that the membrane-bound proteins as attached to cytoskeletal elements deform under varying gravitational conditions, yielding a different three-dimensional cellulose structure.

PROGRESS DURING FY1992

The investigator demonstrated, during KC-135 flights, that the biosynthetic molecules reorientated in varying gravitational conditions, as shown by the splaying effect of the cellulose fibers. Information was published.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Dudlika, K., Cousins, S. K., and Nagy, R. Gravity effects on cellulose assembly. *American Journal of Botany 79* (11): 1247–1258, (1992).

TYPE: Ground
DISCIPLINE: Biotechnology
PROJECT TITLE: ***3-Dimensional Modeling of Human Colon Tissues***
RESPONSIBLE CENTER: JSC **PROJECT IDENTIFICATION:** 674-23-01-05

PRINCIPAL INVESTIGATOR: Dr. J. Milburn Jessup
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TASK OBJECTIVE/DESCRIPTION

The proposal is to study the mechanical decoupling effects of microgravity on cellular interactions.

RESEARCH APPROACH

The investigator utilized a NASA rotating-wall vessel to emulate microgravity—randomizing the gravitational vector and reducing the shear forces. The cellular aggregation and adhesion was thereby facilitated as a result of shear force reduction; high shear can disassociate cellular aggregates. Cellular synergism led to differentiation and higher fidelity in vitro models as compared to the in vivo precursor. Results are based upon micrographs and biochemical tests.

PROGRESS DURING FY1992

The investigator grew adenocarcinoma tissue under simulated microgravity conditions. Several biochemical markers that heretofore were not present in standard tissue culture were expressed. The investigator has extended his work to include normal human colonic development and normal human crypts. Such advances are documented in several publications.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Jessup, J. M., Brown, K., Ishii, S., Ford, R., Goodwin, T. J., and Spaulding, G. F. Simulated microgravity does not alter epithelial cell adhesion to matrix and other molecules. *Molecular Biology of the Cell,* vol. 3, September 1992.

— Jessup, J. M., Brown, K., Ishii, S., Ford, R., Goodwin, T. J., and Spaulding, G. F. "Simulated microgravity does not alter epithelial cell adhesion to matrix and other molecules." American Society for Cell Biology Annual Meeting, Denver, CO, November 1992.

— Jessup, J. M., Ford, R., Goodwin, T. J., and Spaulding, G. F. "Use of microgravity emulation to test the function of three-dimensional human colon carcinoma cell cultures." COSPAR Meeting, Washington, DC, August 1992.

— Jessup, J. M., Ford, R., Goodwin, T .J., and Spaulding, G. F. "Effects of simulated microgravity on human epithelial cell association and recognition." Aerospace Medical Association meeting, Miami, FL, May 1992.

TYPE: Ground
DISCIPLINE: Biotechnology
PROJECT TITLE: *Separation of Chromosome-Size DNA Molecules*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-23-08-12

PRINCIPAL INVESTIGATOR: Dr. Ponzy Lu
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TASK OBJECTIVE/DESCRIPTION

This project addresses the problem of DNA separation by gel electrophoresis. Since we are interested in DNA molecules of 10^6 – 10^8 base pairs in length (10^9 – 10^{11} daltons), or molecules that are polyanions of 2-nm diameter with lengths ranging from millimeters to many centimeters, which distort as they move through the electrophoretic matrix, existing theories and models for electrophoretic transport processes must be modified.

The effort will complement parallel national efforts to map and sequence the entire human genome. There are currently limitations in the human genome project which can be addressed by the technologies to be developed by this research project. Even if the human genome project is completed using existing methods, the technology to be developed here will extend the benefits of those efforts to all biological species, including those used as models of human disease and for agriculture and industry.

The project is an extension of NASA support of electrophoretic-separation process development over the past decade. The extrapolation of currently employed methods for DNA separation suggests the use of more dilute electrophoretic media to allow larger porosity and consequently shorter reorientation times of the polymer subjected to pulsed electric fields. The only method to maintain fluid stability in the presence of chemical and physical density heterogeneity is the microgravity environment. Since the separated DNA will be used for genetic analysis, this program will keep space science applications at the cutting edge of biotechnology.

RESEARCH APPROACH

The investigations will be as outlined in the original proposal, with emphasis on identifying the microgravity component. We have modeled the motion of DNA in Newtonian and non-Newtonian fluids, using thin wire as a mechanical model, with gravitation as the electrical field analog. The results were unexpected and were used to formulate the experiments with DNA. The findings show that the wire falls end first, axis vertical, in the non-Newtonian fluid, and that longer wire falls faster.

In the Newtonian fluid all wire lengths fall at the same rate, horizontally. This latter observation parallels the observations of Olivera, Baine, and Davidson [*Biopolymers* 2, 245–257 (1964)] where DNA of all lengths move at identical velocities in free Newtonian fluids in an electric field.

The apparatus located at the University of Pennsylvania to directly observe the orientation of DNA molecules during the electrophoretic process was built in year 1 of the project and has been used to observe DNA orientation in electric fields typically used for gel electrophoresis. The experiments show considerable DNA orientation on non-Newtonian compared to Newtonian fluids. In fact, the orientation data suggest that the DNA molecular configuration in unrosslinked polyacrylamide is similar to that in conventional agarose electrophoresis. Since our non-Newtonian fluid is a noncrosslinked polyacrylamide, the need for microgravity to prevent convection becomes obvious. Given the length of naturally occurring DNA, the dimensions of the electrophoresis system would need to be measured in meters rather than in centimeters, making Earth-bound stabilization by density gradient less useful, if not useless. An absolute requirement for convectio-free fluid is necessary for resolution in the separation process.

As an alternative matrix for the DNA separation process, glass bead material described in the original proposal was explored. Experiments are in progress to establish that megabase lengths of DNA are indeed electrophoresed gels in the presence of glass beads of 170–200 μ diameters.

PROGRESS DURING FY1992

Direct video imaging of the DNA under the influence of an electric field in Newtonian fluids and non-Newtonian fluids has confirmed the above observation on DNA orientation.

Using the experience over the period of this project, we have designed several experiments to exploit our findings for gel-free separation of DNA. Initial experiments will employ lambda DNA concatomers which are 48 Kb and integral multimers of 48 Kb.

As with all basic research programs, new instrumentation leads to new approaches to existing problems. Our ability to measure DNA helix orientation will allow us to probe rotational diffusion in RNA structures. Of particular interest will be the conformation of ribozymes and regulatory regions of RNA viruses, including HIV. We plan to pursue this during the current year.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Chee, D.-W., Cho, Y. I., Lu, P. Electrophoretic orientation of lambda DNA in viscoelastic solution. For *Nucletic Acids Research*, in preparation, 1992.

— Cho, K., Chee, D.-W., and Cho, Y. I. A study of the length effect on the mobility of a thin cylinder in a free viscoelastic solution. Submitted to the *Journal of non-Newtonian Fluid Mechanics,* 1992.

— Cho, K., Cho, Y. I., and Park, N. A. "Hydrodynamics of large-aspect ratio circular cylinders moving vertically in a viscoelastic fluid" FED. Vol.. 124, 53-58 (1991) presented at the ASME Winter Annual Meeting held in Atlanta, Dec. 1-6, 1991.

— Cho, K., Cho, Y. I., and Park, N. A. Studies on the hydrodynamics of a vertically falling thin cylinder *Journal of non-Newtonian Fluid Mechanics 45,* 105-145, (1992).

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *An Experimental and Theoretical Study of Radiative Extinction of Diffusion Flames*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-29

PRINCIPAL INVESTIGATOR: Prof. Arvind Atreya
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TASK OBJECTIVE/DESCRIPTION

The objective of this program is to quantify the conditions under which a stabilized, laminar diffusion flame will be extinguished by radiative heat losses from flame-generated particulates (e.g., soot) that drain the chemically released energy from the flame.

These tests must be conducted in microgravity because radiation-induced extinction may not be possible under normal-gravity conditions, where buoyancy-generated convection would be swept upward and away from the flame. These flames will demonstrate the concept of radiative extinction in stabilized flames, distinct from the case of spreading diffusion flames.

RESEARCH APPROACH

The program is to have simultaneous experimental and theoretical efforts. Experimentally, normal-gravity tests using a quasi-one-dimensional counterflow diffusion flame burner will be studied to understand soot production and oxidation rates and their optical properties. These data are needed both for the formulation of the reduced-gravity testing and for the development of theoretical models.

Subsequent reduced-gravity testing is to be pursued in the 2.2 second drop tower at NASA Lewis Research Center, where a laminar diffusion flame is to be stabilized about a spherical porous burner. In these tests the local fuel concentrations will be varied by the introduction of inerts into the fuel, flow stream. In these tests, measurements of flame temperatures and radiated flux will be used for comparisons with theory.

A numerical model will be developed to simulate the reduced-gravity experimental configuration, and will include chemical kinetic modeling and modeling for the production and consumption of soot particulates. A model for the radiant emissions from the flame associated with the particulates will be developed.

PROGRESS DURING FY1992

Soot volume fractions, species concentrations, and temperature distributions inside a normal-gravity, counterflow diffusion flame have been measured. Comparisons with theoretical models in the literature have been initiated using soot formation and oxidation rates obtained from the normal-gravity experiments. An apparatus for the planned 2.2-second drop tower tests at NASA Lewis has been designed and fabricated using a spherical porous burner.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Atreya, A., Wichman, I., Guenther, M., Ray, A., and Agrawal, S. "An experimental and theoretical study of radiative extinction of diffusion flames." Pesented to the 2nd International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

— Zhang, C., Atreya, A., and Lee, K. Sooting structure of methane counterflow diffusion flames with preheated reactants and dilution by products of combustion. *Proceedings of the Twenty-fourth International Symposium on Combustion, Sydney, Australia, July 1992.* In preparation, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Ignition and Combustion of Bulk Metals in Microgravity*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-30

PRINCIPAL INVESTIGATOR: Prof. Melvyn C. Branch
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University of Colorado
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TASK OBJECTIVE/DESCRIPTION

The project is an experimental investigation of the mechanisms of ignition and subsequent self-sustained combustion of common metal pellets under low-pressure oxygen atmospheres in a range of gravity fields. Unique features of the research are a radiant ignition source, to eliminate the contamination of the usual promoted igniters, and precise determination of mass change, flame characteristics, surface structure, and temperatures in each phase.

RESEARCH APPROACH

The experiments are conducted with a continuous lamp energy source and instrumentation developed to determine mass loss, surface morphology, flame spectra, and combustion products. Elevated-gravity fields are to be studied in a centrifuge; low-gravity fields are to be studied in an airplane. Concurrent numerical modeling calculations guide the experimental research.

PROGRESS DURING FY1992

Modeling and experiments have been completed with iron, 1018 carbon steel, titanium, copper, and aluminum in normal gravity. Results have demonstrated the feasibility and application of a novel radiant lamp ignition source. The data define the seperate steps of initial heating, ignition, and self-sustained combustion. The numerical modeling has been completed to cover the range of 0g to 10g accelerations.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

— Abbud-Madrid, A., Branch, M. C., Feiresen, T. J., Daily, J. W., and Fiechtner, G. J. "A study of the ignition phenomena of bulk metals by radiant heating." For the Sixth International Symposium on Flammability and Sensitivity of Materials in Oxygen-Enriched Atmospheres, ASTM Committee G-4, to be held in the Netherlands, May 1993, submitted 1992.

— Branch , M. C., Abbud-Madrid, A., Feireisen, T. J., Daily, J. W., and Fiechtner, G. J. "A study of the ignition phenomena of bulk metals by radiant heating." Paper presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.

— Feireisen, T. J., Branch, M. C., Abbud-Madrid, A., and Daily, J. W. "Gravitational and pressure effects on the heat-up rate of metal test specimens in a pure oxygen atmosphere." Paper submitted to the 1993 ASTM Committee G-4 Symposium cited above, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Modeling of Microgravity Combustion Experiments*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-31

PRINCIPAL INVESTIGATOR: Prof. John C. Buckmaster
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TASK OBJECTIVE/DESCRIPTION

Modeling plays a vital role in providing physical insights into the behavior revealed by experiment. The program at the University of Illinois is designed to improve our understanding of basic combustion phenomena through the analytical and numerical modeling of a variety of configurations undergoing experimental study in NASA's microgravity combustion program.

RESEARCH APPROACH

Experimental results amenable to modeling are identified and modeling is carried out. This is done in close collaboration with the experimentalist where possible.

PROGRESS DURING FY1992

The most significant accomplishment in FY 1992 is the first numerical calculation of stationary flame-ball structure in hydrogen-air mixtures, and the identification of a lean flammability limit of .0866 (equivalence ratio). This work probably marks the first time a flammability limit computed using detailed submodels has been directly and meaningfully compared to experiments without simplifying assumptions, extrapolations, or artificial ingredients.

Substantial progress has been made in our studies of acoustic instabilities in particle-cloud flames. Of particular significance is work on spherical flames, since this is a configuration under study in the two experimental programs of John Lee and Paul Ronney.

In flame-ball experiments carried out in mixtures containing significant amounts of SF_6, it is believed that the combustion field absorbs a significant amount of its own radiation, and we have devised a model that accounts for this which can be analyzed.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Buckmaster, J. "Analytical and numerical modeling of flame-balls in hydrogen/air mixtures." Presented at the 45th Meeting of the Division of Fluid Mechanics of the American Physical Society, 1992.

— Buckmaster, J. A flame-string model and its stability. *Combustion Science and Technology, 84*, 163 (1992).

— Buckmaster, J. "Modeling of microgravity combustion experiments." Presented at the University of Oklahoma, the University of Houston, Texas A&M University, and the South-West Research Institute, a Southwest Mechanics Lecture Tour, 1992.

— Buckmaster, J. The structure and stability of laminar flames. Accepted for vol. 25 of *The Annual Review of Fluid Mechanics*, 1992.

— Buckmaster, J., and Clavin, P. An acoustic-instability theory for particle-cloud flames. In *Proceedings of The 24th International Symposium on Combustion, July 1992, Sydney, Australia,* In preparation, 1992.

— Buckmaster, J., Gessman, R., and Ronney, P. The three-dimensional dynamics of flame-balls. In *Proceedings of The 24th International Symposium on Combustion, July 1992, Sydney, Australia.* In preparation, 1992.

— Buckmaster, J., and Joulin, G. Influence of boundary-induced losses on the structure and dynamics of flame-balls. *Combustion Science and Technology.* In press, 1992.

— Buckmaster, J., and Lee, C. J. The effects of confinement and heat loss on outwardly propagating spherical flames. In *Proceedings of The 24th International Symposium on Combustion, July 1992, Sydney, Australia,* In preparation, 1992.

— Buckmaster, J., Smooke, M., and Giovangigli, V. Analytical and numerical modeling of flame-balls in hdrogen-air mixtures. Accepted fo,*Combustion Science and Technology.* 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Gravitational Effects on Premixed Turbulent Flames: Studies of the Dynamics of Wrinkled Laminar Flames in Microgravity*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-32

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PHONE:

TASK OBJECTIVE/DESCRIPTION

The objective of the experimental program is to investigate low-Reynolds-number premixed turbulent flames in microgravity to gain a fundamental understanding of the gravitational effects on flame-turbulence interaction processes. This aspect of turbulent flame propagation is not well understood and has yet to be considered in current turbulent combustion theories. Our experimental results are expected to provide guidance and validation for the development of turbulent combustion models to include the effects of gravity.

RESEARCH APPROACH

The experimental work is focused on developing the methodology, experimental apparatus, and laser diagnostics for application in the NASA Lewis Research Center 2.2 drop tower. Flow visualization techniques coupled with computer-controlled image processing are used to characterize the behavior of the aerodynamic flowfield and mean flame properties under microgravity.

To provide the necessary scientific background for the microgravity experiments, a parallel study of laminar and turbulent flames subjected to +g (upwards) and -g (downward) forces is also conducted. These +g and -g laboratory flames are investigated with the use of more sophisticated laser diagnostics such as laser Doppler anemometry to obtain statistical data.

PROGRESS DURING FY1992

A 2.2-second drop tower rig was constructed and tested. The behavior of laminar and turbulent Bunsen type premixed flames under microgravity has been observed by the use of laser schlieren. This is the first successful application of the schlieren technique to microgravity research in the 2.2-second drop tower. The schlieren images are recorded on videotape and are analyzed by computer-controlled image processing. Comparison of the microgravity results with those observed under

normal gravity shows that gravity affects flame propagation through the coupling of the flame dynamics and the surrounding flowfield. Under normal gravity, buoyancy- driven flow instabilities are shown to induce flame flickering. In microgravity, the instability is absent and is not dominant in inducing flame motion.

However, the laminar flames still exhibit some flame instability which is small compared to the normal-gravity flames flickering. In the turbulent flames due to the random nature of the wrinkled flame fronts, the differences between normal and microgravity flames are more difficult to identify and quantify. The differences will be investigated using the appropriate image analysis and display software for characterizing the flame wrinkle scales and their evolution. This work is in progress and the results will be forthcoming.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kostiuk, L. W., Zhou, L., and Cheng, R. K. The effect of gravity on wrinkled laminar flames. *Proceedings of the Second International Workshop on Microgravity Combustion, Cleveland, OH, September 15–17,1992.*

— Kostiuk, L. W., Zhou, L., and Cheng, R. K. "The effect of gravity on wrinkled laminar flames." Poster No. 102, Twenty-fourth Symposium (International) on Combustion, Sydney, Australia, July 5–11, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Combustion of Interacting Droplet Arrays in a Microgravity Environment***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-33

PRINCIPAL INVESTIGATOR: Dr. Daniel Dietrich
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TASK OBJECTIVE/DESCRIPTION

This research program involves the study of one-and two-dimensional arrays of droplets in a buoyant-free environment. The purpose of the work is to extend the data base and theories that exist for single droplets into the regime where droplet interactions are important. The eventual goal being to use the results of this work as inputs to models on spray combustion, where droplets seldom burn individually; instead the combustion history of a droplet is strongly influenced by the presence of the neighboring droplets.

RESEARCH APPROACH

The emphasis of the present investigation is experimental, although comparison will be made to existing theoretical and numerical treatments when appropriate. Both normal-gravity and low-gravity testing will be employed, and the results compared.

The normal-gravity testing will utilize the classical suspended droplet technique; single droplets and droplet arrays will be supported on 125 µm optical fibers in a combustion chamber where the ambient environment can be controlled. The low-gravity testing will employ droplets suspended on 15 µm Si-C fibers, a new technique developed during the past year, again in a combustion chamber where the ambient environment can be changed.

PROGRESS DURING FY1992

The design and construction of the normal-gravity combustion chamber is complete. The chamber has been used for a number of single droplet and droplet array combustion studies. One of these studies was to evaluate the suitablility of an intensified array camera to image the flame in the ultraviolet region of the spectrum as opposed to the visual image usually obtained. The intensified array camera offers the potential to image the OH in and near the flame zone. Intensified-array ultraviolet images were compared to visual images of the flame.

In other studies, single droplets of methanol and n-decane were burned in high-oxygen, low-pressure environments. For pressures of 0.2 - 0.3 atm, microexplosions were observed for the pure fuel droplet. Initial work was also started on burning multiple droplets.

The major development in reduced-gravity droplet combustion has been in the use of very small 15 μm Si-C fibers to support the droplets. These fibers are an order of magnitude smaller that the fibers used in most suspended-droplet studies. Using these fibers also offers the potential to perform temperature measurements in the gas phase surrounding the burning droplet. A new drop-tower apparatus using this new fiber technology has been designed and constructed.

GRADUATE STUDENTS: 0   **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Dietrich, D. L., and Haggard, J. B. "Combustion of interacting droplet arrays in a microgravity environment." Presented at the Second International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Combustion of Electrostatic Sprays of Liquid Fuels in Laminar and Turbulent Regimes*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-34

PRINCIPAL INVESTIGATOR: Prof. Alessandro Gomez
AFFILIATION: Yale University
MAILING ADDRESS: Yale University
Department of Mechanical Engineering
Yale University
New Haven, CT 06520
PHONE:

TASK OBJECTIVE/DESCRIPTION

This research is a combination of theoretical and computational work by Professors Alessandro Gomez (PI, experimental), Marshall B. Long (Co-I, diagnostics) and Mitchell D. Smooke (Co-I, computational), all from Yale University. It involves studying the formation and burning of electrosprays of liquid fuels at both normal and reduced gravity.

Electrosprays are being studied because they offer several advantages over conventional fuel sprays such as (a) generation of a relatively narrow droplet-size distribution; (b) elimination of droplet coalescence and the production of a relatively uniform spray due to the self-dispersion property of the spray; and (c) the possibility of manipulating droplet trajectories.

RESEARCH APPROACH

During the first year of the program the experimental apparatus was built and its performance characterized. Also in the first year testing began on laminar sprays in the counterflow configuration in normal gravity. In subsequent years the laminar counterflow configuration will be tested in zero gravity in the drop towers, and testing will also begin on turbulent spray flames.

PROGRESS DURING FY1992

The project has developed along two parallel avenues: We have performed a variety of cold flow experiments aimed at examining the fundamental mechanism of electrospray atomization and dispersion as well as identifying and characterizing the domain of operating variables under which the generated droplets are quasi-monodisperse; and another focus of the research has been on the combustion of the electrospray in the laminar regime. A counterflow spray burner has been constructed and tested at normal gravity. The dynamics of the interaction between the droplets and the flame have been examined.

Primary diagnostic tools being used are a commercial phase Doppler anemometer (PDA), the workhorse of this phase of the project. It is used to measure distributions of droplet size and either axial or radial velocity component; and a shadow graph system consisting of a nanosecond flashlamp, a long-range microscope, and a charged-coupled device camera (CCD), capable of capturing and digitizing images of droplet shadows with an overall magnification of up to 1100X. Further details are given in the six publications (listed below) that have resulted from the research activity in the first seventeen months of the project. Two graduate students are involved in the project.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Chen, G., and Gomez, A., Counterflow diffusion flames of quasi-monodisperse electrostatic sprays. *Twenty-fourth Proceedings of the Sumposium International on Combustion,* The Combustion Institute. In preparation, 1992.

— Gomez, A., and Chen, G. Secondary atomization in the combustion of electrostatic sprays. Submitted to *Combustion and Flame* , 1992.

— Gomez, A., and Tang, K., Fission of charged droplets in electrostatic sprays. Submitted to *Phys. Fluids A* , 1992.

— Gomez, A., and Tang, K. Stability domain of an electrospray generating monodisperse droplets in the size range 1-140 µm. Accepted for *J. Aerosol Sci.,* 1992.

— Gomez, A., and Tang, K. *Proceedings of the fifth international conference on liquid atomization and Spray Systems, ICLASS-91, Gaithersburg, MD, USA,* H. G. Smerjian, ed., NIST Special Publication No. 813, p. 805, 1991.

— Tang, K. and Gomez, A. On the structure of an electrospray of monodisperse droplets. Submitted to *Phys. Fluids A* , 1992.

Type: Ground
Discipline: Combustion Science
Project Title: *Structure and Dynamics of Premixed Flames in Microgravity*
Responsible Center: LeRC **Project Identification:** 674-22-05-22

Principal Investigator: Dr. K. Kailasanath
Affiliation: Naval Research Laboratory
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Task Objective/Description

The objective of this research is to investigate fundamental problems in the combustion of premixed gases, such as the differences in the propagation and extinction of gas-phase flames in normal and microgravity and the structure and stability of burner-stabilized flames.

Research Approach

We study the structure and dynamics of premixed flames by performing detailed numerical simulations using time-dependent, one- and two-dimensional numerical models. These models solve the multispecies coupled partial differential reactive-flow equations.

The models include detailed chemical-kinetics mechanisms, algorithms for thermal conduction, molecular diffusion, viscosity, heat conduction to walls, convective and radiative transport, and effects of gravity. We also plan to use reduced-chemistry models after they have been validated or calibrated against detailed models.

Progress During FY1992

The detailed dynamics of the extinguishment of downward-propagating hydrogen-air flames have been simulated. These simulations indicate that both gravity and heat losses to the walls are simultaneously required to cause the observed extinguishment. The actual mechanism of extinguishment has been identified to be the dilution of the unburned mixture with the products of combustion caused by the recirculatory flow set up near the walls by the buoyant forces. The calculated lean-flammability limit is in good agreement with experiments. Furthermore, the above mechanism of extinguishment seems to explain the extinguishment of other fuel-air mixtures also (during downward propagation).

The relative roles of hydrodynamic and thermo-diffusive effects for hydrogen flames have been further clarified. In earlier simulations rich hydrogen-oxygen-

nitrogen (3:1:16) flames have been found to be flat in 2-and 5.1-cm-wide systems even in zero-gravity, while simple theory would predict them to be nonplanar owing to the hydrodynamic instability. When the system size was increased to 9 cm, the flame was indeed found to develop a curved structure due to hydrodynamic effects. Even this curvature is suppressed if gravity effects (downward) are turned on. What these results imply is that, except for very large systems (system size or flame thickness greater than about 20), the diffusive transport effects dominate over the hydrodynamic effects in hydrogen systems. Whether this is true for hydrocarbon systems needs to be investigated.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kailasanath, K., Patnaik, G., and Ganguly, K. Dynamics of flames near the rich-flammability limit of hydrogen-air mixtures. Accepted for publication in *Progress in Aeronautics and Astronautics*, June 1992.

— Kailasanath, K., Patnaik, G., and Oran, E. S. "Structure and dynamics of premixed flames in microgravity." 2nd International Microgravity Combustion Workshop, Cleveland, OH., September 1992.

— Patnaik, G., and Kailasanath, K. "Detailed transient two-dimensional simulations of laminar flame structures in lean hydrogen-air mixtures." Presented at the 4th International Conference on Numerical Combustion, St. Petersburg, FL, December 1991.

— Patnaik, G., Kailasanath, K., and Oran, E. S. Effect of gravity on flame instabilities in premixed gases. *AIAA Journal*, vol. 29, no. 12, pp. 2141–2148, (November 1991).

— Patnaik, G. and Kailasanath, K. "On the extinguishment of downward propagating hydrogen-air flames." Presented at the Fall Technical Meeting of the Eastern Section of the Combustion Institute, Orlando, FL, October 1991.

— Patnaik, G., and Kailasanath, K. "Lean flammability limit of downward propagating hydrogen-air flames." Presented at the AIAA 30th Aerospace Sciences Meeting, Reno, NY, January 1992. Also AIAA Paper 92-033G, AIAA, Washington, DC, 1992.

— Patnaik, G., and Oran, E. S. "Parallel processing for combustion modeling applications." Presented at the IEEE Scientific Supercomputing Meeting, Washington, DC, April 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Radiative Ignition/Subsequent Flame Spread of Cellulosic Fuels in Microgravity*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-35

PRINCIPAL INVESTIGATOR: Dr. Takashi Kashiwagi
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TASK OBJECTIVE/DESCRIPTION

This project models and solves numerically, with experimental verifications, the two- and three-dimensional, time-dependent relationships of ignition and flame spread for paper ignited by radiant energy in a microgravity environment. Processes to be modeled include the endothermic surface pyrolysis, the exothermic surface (char) oxidation, and the exothermic gas-phase combustion. Variations to model realistic situations include thermally thin and thick fuels and quiescent and air-flow conditions.

RESEARCH APPROACH

Numerical models are developed, with experimentally determined properties and reaction rates, to predict the time-dependent radial contours of temperature, density, velocity, and chemical species in the gas phase during the steps of ignition, pyrolysis, and subsequent flame spread. Verifying experiments are defined for ground-based and flight microgravity facilities.

PROGRESS DURING FY1992

The numerical models for all the quiescent, thin-fuel cases have been completed, with output in the form of plots of the temperature, density, velocity, and specie contours at fractional second intervals during the first 10 seconds of the combustion history.

Important findings are that the paper fuel will not transition to flame spread for quiescent, microgravity air (21% O_2) environments. A quiescent atmosphere of at least 50% O_2 or air flow at lower oxygen-concentration atmospheres, is required for the transition. Independent, small-scale ground-based experiments verified the qualitative conclusions.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kashiwagi, T., and Nambu, H. F. Global kinetic constants for thermal oxidative degradation of cellulosic paper. *Combustion and Flame* , vol. 88, pp. 345–368, (1992).

— Kushida, G., Baum, H. R., Kashiwagi, T., and di Blasi, C. Heat and mass transport from thermally degrading thin materials in a microgravity environment. *Journal of Heat Transfer*, vol. 114, pp. 494–502, (1992).

— Nakabe, K., Baum, H. R., and Kashiwagi, T. "Ignition and subsequent flame spread over a thin cellulosic material." Paper presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.

— Yamashita, H., Baum, H. R., and Kashiwagi, T. "Heat and mass transport from heated material in a low reynolds number microgravity environment." Paper presented at the Fourth International Conference on Numerical Combustion, SIAM, December 1991.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Measurements and Modeling of Sooting Turbulent Jet Diffusion Flames Under Normal and Reduced-Gravity Conditions*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-36

PRINCIPAL INVESTIGATOR: Prof. Jerry C. Ku
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TASK OBJECTIVE/DESCRIPTION

The objectives of this study are to model soot formation and radiation for turbulent jet diffusion flames, and to determine the modeling coefficients from measured data, under both normal and reduced-gravity conditions. Microgravity combustion is not only relevant to fire safety on board a spacecraft but also provides a unique condition for better understanding of the combustion fundamentals.

RESEARCH APPROACH

In regard to experimental measurements, thermophoretic particle sampling and electron microscopy are used for soot particle size and aggregate morphology analysis. Laser light absorption imaging provides for the determination of soot-volume fractions, and emission imaging and thermocouple measurements will be used for soot thermometry. Laser Doppler velocimetry may possibly be employed to measure velocities and turbulence intensities, but is beyond the stated deliverables of this effort.

In the area of modeling, Favre-averaged boundary layer equations with a k-ε-g turbulence model and the conserved scalar approach with an assumed β-pdf (probability density function) are used to predict flow field and gaseous species mole fraction profiles, respectively. Transport of soot particles is described by equations for volume fraction and number density using rate equation models. The energy equation is included to provide coupling between flame structure and radiation analyses. The radiative flux is solved from the radiative transfer equation (RTE).

PROGRESS DURING FY1992

Both the techniques of thermophoretic sampling and imaging light extinction have been successfully demonstrated in the laboratory. A 2.2-second drop package has been designed and constructed to implement these measurements in the 2.2-second drop tower facility.

Soot particle size and aggregate morphology data have been obtained for laminar flames under reduced- gravity conditions. It has been observed that soot aggregates in reduced-gravity flames have larger numbers of primary particles and larger primary particle size than those under normal gravity conditions. This is thought to be due to longer residence times associated with reduced-gravity flames, which have a smaller axial velocity owing to the absence of buoyant forces. A burner for turbulent studies is presently being constructed.

Results from the modeling effort compare well with published data, and accurate predictions are obtained for flame structure and soot volume fraction. A third-order spherical harmonics (P_3) approximation has been applied to solve the RTE. Some numerical problems have been experienced in solving the resulting elliptic partial differential equations. To provide comparisons, other approaches for solving the RTE are being considered.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ku, J. C. Measurements and prediction of soot particles in laminar jet diffusion flames under normal and reduced gravity conditions. For *Combustion and Flame*. In preparation, 1992.

— Ku, J. C. A P_3 approximation for radiative transfer from soot particles in axisymmetric diffusion flames. For *J. Heat Transfer*. In preparation, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Studies of Flame Structure in Microgravity***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-37

PRINCIPAL INVESTIGATOR: Dr. Chung K. Law
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TASK OBJECTIVE/DESCRIPTION

The objectives of this work are to understand and quantify the structure, stabilization mechanisms, soot formation in, and extinction of one-dimensional premixed and nonpremixed laminar flames.

This work takes advantage of the microgravity environment to obtain nonplanar, one-dimensional flames that are stabilized around curved burners in the absence of buoyant or externally imposed flows. This flame configuration is a more fundamental flame paradigm than can be established in a normal-gravity environment, providing stabilized flames with minimal nonadiabaticities and without aerodynamic straining.

RESEARCH APPROACH

This program comprises three main elements. A numerical simulation of one-dimensional laminar flames is to be developed that, in addition to including the usual fluid mechanical and heat transfer mechanisms, will include detailed chemical kinetic mechanisms for comparison with the unique experimental results. A drop-tower test apparatus is to be used to observe premixed laminar flames stabilized about a cylindrical and then a spherical porous burner to distinguish heat loss and flow divergence influences upon the flame stabilization and flamefront stability. A drop-tower apparatus is to be used to observe nonpremixed laminar flames stabilized about the cylindrical and spherical burners to study soot formation, gas-phase unsteadiness, kinetic extinction, and radiative extinction.

PROGRESS DURING FY1992

During this year's work an improved cylindrical burner was developed for tests in the NASA LeRC 2.2-second drop tower. A series of tests using mixtures of methane, oxygen, nitrogen, and helium were completed. Helium was included to (a) reduce the flame temperature, thereby supressing hydrodynamic flamefront instability, (b) increase the Lewis number of the flame, thereby supressing thermo-diffusive flamefront instability, and (c) reduce the laminar flame speed in order to stabilize

the flame at larger standoff distances from the burner, thereby reducing heat losses to the burner. Substantial improvments in flame uniformity were observed compared to the first cylindrical burner used during the previous year. Based upon the analysis of these tests the burner design has again been modified for additional 2.2-second drop tower tests.

The Sandia flame code was modified for use with the cylindrical geometry and was used to compare the numerically calculated flame response with the microgravity flames observed experimentally. Although trends with flow velocities and mixture ratios are the same, the computed flame location is larger than observed experimentally. Separately, an asymptotic analysis of cylindrical flames has been developed.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Eng, J. A., Egolfopoulos, F. N., and Law, C. K. On the dual response and surface recombination in burner-stabilized flames. *Proceedings of the 27th National Heat Transfer Conference, Minneapolis, MN*; ASME-HTD vol. 166, 1991.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *A Fundamental Study of the Combustion Syntheses of Ceramic-Metal Composite Materials Under Microgravity Conditions*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-38

PRINCIPAL INVESTIGATOR: Prof. John J. Moore
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MAILING ADDRESS: Department of Metallurgical and Materials Engineering
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TASK OBJECTIVE/DESCRIPTION

The objectives of the proposed research program are concerned with obtaining a thorough scientific understanding of the effects of microgravity on the in-situ synthesis of ceramic matrix-metal composite materials, using a novel and innovative mode of combustion synthesis reaction.

RESEARCH APPROACH

An exothermic combustion reaction will be used to provide a porous ceramic-ceramic matrix which is simultaneously infiltrated with excess liquid aluminum from the combustion reaction. The research will investigate the underlying fundamental mechanistic differences between conducting these combustion synthesis reactions under normal gravity and low-gravity conditions.

PROGRESS DURING FY1992

The main thrust of this research has been to investigate the principle of synthesizing ceramic-metal composites using combosition synthesis techniques under 1-g conditions. Results and phenomena have been identified such that appropriate reaction systems can now be utilized under microgravity conditions in order to fully assess the implications of microgravity on the synthesis of ceramic-metal composite materials.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Combustion Research***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-08

PRINCIPAL INVESTIGATOR: Dr. Howard Ross
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PHONE: (216) 433-2868

TASK OBJECTIVE/DESCRIPTION

The task objective is to advance an understanding of fundamental combustion phenomena and/or processes that are affected by the presence or absence of gravity.

RESEARCH APPROACH

The research approach is to provide for limited precursor studies by external investigators and for the engineering and fabrication of hardware needed to conduct in-house research and assist in the research efforts conducted on-site at LeRC in support of Code SN-sponsored principal investigators (PIs) and National Research Council (NRC) graduate student researchers. Funds for facility overhead charges are provided through separate Research and Technology Operations Plans (RTOP) resources.

PROGRESS DURING FY1992

Dr. D. Dietrich of Sverdrup Technology, Inc. assisted in the development of the Glovebox flight hardware development, verification, crew training, and mission support. In addition, he and a student completed a few drop-tower tests in H. Ross's laser rig, showing the influence of gravity on the convective flow around a candle flame. He also continued to pursue candle-flame modeling, developing with Prof. T'ien of Case Western Reserve University (CWRU) a model for the wick dynamics. Finally, considerable time was spent by D. Dietrich in support of the Japanese/UCSD high-pressure droplet vaporization study and the droplet combustion experiment of Profs. Williams and Dryer. The former support resulted in the draft article with Prof. Williams and Dr. Sato on the drop-tower results, which was presented in a poster session at the 24th Symposium on Combustion and then accepted as an article to *Combustion Science and Technology*.

Dr. U. Hegde of Sverdrup completed a theoretical study of flame-acoustic interactions related to the "chattering flame" phenomenon observed in particle cloud experiments. With L. Facca and Dr. Ross, he compared the theory to the experiment, and documented it in a paper that also will be published in

Combustion Science and Technology. He also assisted in the development of the updated "Program Overview" on microgravity combustion science, and helped monitor the grant with Prof. Buckmaster. In order to accelerate the publication date of the document, $2,000 was expended for overtime hours in the Graphics and Editorial department.

Funds were also expended on miscellaneous equipment such as film development, personal computers, A/D and I/O boards, thermocouples, thermistors, transducers, mass flow controllers, video cameras, bottled gases regulators, translation stages, optical breadboards, etc, in support of several 1-g and drop-tower investigations.

Additionally in-house support was provided to other visiting researchers (Premixed Gas Combustion by Princeton, High Pressure Drop. Combustion by Japanese/UCSD, Turbulent Premised Gas Studies by R. Cheng/LBL; Flame Curvature Effects by C. K. Law/Princeton, etc.) and those on no-cost time extensions; this support consists typically of purchasing of bottled gases, regulators, portable PC's, fabrication services, etc. Finally, in-house support of the Combustion Science Discipline Working Group (DWG) and review committees will be provided.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Hegde, U., Ross, H. D., and Facca, L. T., Longitudinal mode instabilities of particle cloud combustors in a low gravity environment. To appear in *Combustion Science and Technology*, 1992.
— Jackson, G. S., Avedisian, C. T., and Yang, J. C., Observations of soot during droplet combustion at low gravity: heptane and heptane/monochloroalkane mixtures. *Int. J. Heat Mass Transfer*, vol. 35, no. 18, pp. 2017–2033 (1992).
— Microgravity Combustion Group. Microgravity combustion science: prog- ress, plans, and opportunities. NASA Technical Memorandum 105410; April 1992.
— Mikami, M., Kono, M., Sato, J., Dietrich, D. L. and Williams, V. Combustion of miscible binary-fuel droplets at high pressure under microgravity. Accepted by*Combustion Science and Technology*, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *Combustion Experiments in Reduced Gravity with 2-Component Miscible Droplets*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-39

PRINCIPAL INVESTIGATOR: Prof. Benjamin Shaw
AFFILIATION: University of California, Davis
MAILING ADDRESS: Department of Mechanical, Aeronautical & Materials Engineering
University of California, Davis
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PHONE:

TASK OBJECTIVE/DESCRIPTION

The objective of this investigation is to study the combustion characteristics of miscible, binary droplets initially in the millimeter-size range, in a low-gravity environment. The fuel mixture components are selected to provide significant variations in component volatilities (e.g., heptane and hexadecane). Specifically, experimental data on transient droplet diameters (including two-stage combustion and droplet disruption), transient flame behavior (including sudden flame contraction and extinction), and transport of soot particles will be obtained using ground-based low-gravity facilities.

RESEARCH APPROACH

Binary, miscible fuel droplets will be deployed in a low-gravity environment and ignited. High- speed films of both the droplet size as well as the flame position will be obtained. These high-speed films will be analyzed frame by frame using digital image analysis techniques to obtain droplet burning rates, and flame positions as a function of time. Any other phenomenon, such as microexplosion or soot particle transport, will also be recorded for analysis and interpretation. All the experiments will be performed using an experimental rig similar to the Droplet Combustion Experiment rig at NASA Lewis Research Center in the 2.2-second drop tower.

PROGRESS DURING FY1992

During the early part of 1992 preliminary tests were conducted using heptane/hexadecane mixtures in the 2.2-second drop tower. Following these tests some improvements were to the test cell; specifically a small Si C fiber of 10–15 micron diameter was added to support the droplet after deployment. More low-gravity data were collected during July 1992 using the Lewis Droplet Combustion rig with heptane/hexadecane mixtures in CO_2/O_2 atmosphere and air.

Currently, a drop rig similar to the Lewis rig is being designed and built at the University of California, Davis, with a number of improvements based on the

lessons learned during the first phase of testing. It is expected that this will be used to obtain further test data at the 2.2-second drop tower in the near future.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Shaw, B. D., and Aharon, I. "Combustion experiments in reduced gravity with two-component miscible droplets." Presented at the Second International Microgravity Combustion Workshop, Cleveland, OH, August 31, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: ***Combustion of Solid Fuel in Very Low Speed Oxygen Streams***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-25

PRINCIPAL INVESTIGATOR: Prof. James T'ien
AFFILIATION: Case Western Reserve University
MAILING ADDRESS: Department of Mechanical &
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PHONE:

TASK OBJECTIVE/DESCRIPTION

The objective of this program is to understand the mechanisms that control the spreading of flames and the flammability of materials in low-speed oxidizing flows, including buoyantly driven concurrent and opposed flows and forced-concurrent flows.

This work, comprising both theoretical and experimental components, attempts to provide a fundamental understanding of the practical flame-spreading environment that exists between the normal-gravity, buoyantly dominated environment, where flow velocities are much larger than flame spreadrates, and the quiescent microgravity environment, where the only flow relative to the flame is the flame-spreading velocity into fresh oxidizer. Additionally, this work will attempt to distinguish between influences of buoyantly induced flows and flows that are externally imposed.

RESEARCH APPROACH

The work consists of three major components. A numerical simulation of the concurrent-flow flame-spreading process is to be developed that accounts for both the stabilization of the flame at the leading edge facing the flow and the downstream tip of the flame where the flame spreading occurs. The required computational domain must therefore be large in comparison to the opposed-flow case. A steady solution will be sought, but a transient model is to be developed. Concurrent-flow spreading and flammability experiments are to be conducted in low-speed forced flows in both of the NASA Lewis drop towers. An aircraft apparatus is to be developed to obtain flame-spreading data, both upward and downward, in partial gravity between 0.01g and 0.6g.

PROGRESS DURING FY1992

During 1992 a steady numerical simulation of concurrent-flow flame spreading was completed. The two-dimensional, elliptic conservation equations for mass, momentum, energy, and chemical species were used in the flame stabilization zone.

Parabolic equations can be applied at an appropriate location downstream, and were used instead of the more difficult elliptic equations. A significant effort was made to determine the appropriate transition point between the elliptic and parabolic regions and to ensure the continuity of the computed results across the boundary. The effect of flow velocity and oxygen concentration at zero gravity was investigated for thin fuels, and steady solutions were obtained. Computed detailed flame structures get larger and spread faster as flow velocity or oxygen concentration increases. Both flame quenching, at the lowest flow velocities, and blowoff extinction, at the highest flow velocities, have been numerically simulated. Subsequent modifications will incorporate unsteady flame spread and gas-phase radiation.

A second series of 2.2-second drop tower tests observing concurrent-flow flame spreading and flammability limits was initiated using the combustion tunnel in which improved control over the experiment ignition energy was implemented. Most of these tests showed flame growth during the 2.2-second test time, rather than steady flame spreading. As the unsteady numerical modeling develops, these results will be compared with theory. Development of a new device for studying flames in flow velocities below those obtainable in the combustion tunnel was initiated.

An aircraft apparatus, capable of flight on either of the NASA reduced-gravity aircraft, was completed and flown during each of five weeks on the KC-135 at the Johnson Space Center. During these flights, a complete flammability map was obtained for downward burning over acceleration ranges from 0.05g to 0.6g. These tests demonstrated increased downward flammability at reduced-gravity levels compared to both the zero- and normal-gravity cases. Upward flame spreading tests showed significant downstream hydronamic unsteadiness at all gravity levels tested in normal atmospheric pressure. A small number of tests at reduced pressure were performed to capture cases without this unsteadiness, and in so doing determined estimates of pressure related flammability limits over a range of oxygen/nitrogen mixtures.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Ferkul, P. V., and T'ien, J. S. "A model of low-speed concurrent-flow flame spread over a thin solid fuel." Presented at the Annual Conference on Fire Research, NIST, Gaithersburg, MD, October 1992.

— T'ien, J. S., Sacksteder, K. R., and Ferkul, P. V. "Combustion of solid fuel in very-low speed oxygen streams." Presented to the 2nd International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

TYPE: Ground
DISCIPLINE: Combustion Science
PROJECT TITLE: *High Pressure Droplet Combustion Studies*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-22-05-41

PRINCIPAL INVESTIGATOR: Prof. Forman A. Williams
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TASK OBJECTIVE/DESCRIPTION

This is a joint research program, pursued by investigators at the University of Tokyo, University of California, San Diego, and the NASA Lewis Research Center. The focus is on high-pressure combustion of miscible binary fuel droplets. It involves construction of an experimental apparatus in Tokyo, mating of the apparatus to a NASA-Lewis 2.2-second drop tower in Cleveland, with experimental results analyzed jointly by the Tokyo, UCSD, and NASA investigators. The project was initiated in December, 1990, and has now involved three periods of drop-tower testing by Mr. Masato Mikami at Lewis.

RESEARCH APPROACH

The research accomplished thus far concerns the combustion of individual fiber-supported droplets of mixtures of n-heptane and n-hexsadecane, initially about 1 mm in diameter, under free-fall microgravity conditions. Ambient pressures ranged up to 3.0 MPa, extending above the critical pressures of both pure fuels, in room-temperature nitrogen-oxygen atmospheres having oxygen mole fractions, X, of 0.12 and 0.13. The general objective is to study near-critical and super-critical combustion of these droplets and to see whether three-stage burning, observed at normal gravity, persists at high pressures in microgravity.

PROGRESS DURING FY1992

The objective of this research is to study near-critical and super-critical combustion of droplets consisting of binary fuel mixtures. Experimental results are reported on the burning of fiber-supported droplets of mixtures of n-heptane and n-hexadecane, initially about 1 mm in diameter, under free-fall microgravity conditions.

The ambient pressures range up to 3.0 MPa, extending above the critical pressure of both fuels, in room-temperature nitrogen-oxygen atmospheres having oxygen mole fractions of 0.12 and 0.13. Three-stage burning of the binary fuel droplets is observed, and the onset time of the second stage is compared with the predictions of an existing theory. Experimental evidence of thermo-capillary and/or diffuso-

capillary convection during the droplet burning is obtained. The results contribute to improving understanding of binary-fuel droplet-combustion processes at high pressures. One graduate student from the Universtiy of Tokyo is involved in the program.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

— Mikami, M., Kono, M., Sato, J., Dietrich, D. L., and Williams, F. A. Combustion of miscible binary-fuel droplets at high pressure under microgravity. Poster presented at the Twenty-Fourth Symposium (International) on Combustion, The Combustion Institute, 1992; Accepted for *Combustion Science and Technology* , 1992.

Type: Ground
Discipline: Electronic Materials
Project Title: *Growth of Zinc Selenide Single Crystals*
Responsible Center: MSFC **Project Identification:** 674-21-08-06

Principal Investigator: Prof. Elmer E. Anderson
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Task Objective/Description

To determine the optimum growth conditions for obtaining single crystals of ZnSe and ZnS of good optical quality.

Research Approach

Crystals will be grown by the physical vapor transport method using a three-zone travel furnace.

Progress During FY1992

Growth of mixed crystals of ZnSe and ZnS has been undertaken in an attempt to get a better understanding of the principal cause of dislocation formation. Progress has been made on three-dimensional modeling of the transport rate.

Graduate Students: 1 **Degrees Granted:** 0

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Memory Effects in the Organometallic Chemical Beam Epitaxy of Compound Semiconductors*
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** 674-21-06-06

PRINCIPAL INVESTIGATOR: Dr. Klaus J. Bachmann
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TASK OBJECTIVE/DESCRIPTION

The goal of this research program is the improvement of the control of the composition of compound semiconductor heterostructures under the conditions of chemical beam epitaxy (CBE) and related low-pressure chemical vapor deposition. The linkage to NASA's mission is the opportunity for containerless processing in space, which is expected to eliminate memory effects. Under ground-based conditions, memory effects are caused by the adsorption on the walls of the vacuum chamber and the pumping system of precursor molecules and reaction products, ejected from the surface of the semiconductor heterostructure. Their uncontrolled, slow release during later stages of epitaxial sequencing introduces impurities into the epilayers that degrade their properties.

Since safety concerns with regard to the transport of highly toxic and pyrophoric source materials currently prohibit experimentation in the containerless vacuum environment of space, an important aspect of this research program is the replacement of hazardous liquid and gaseous sources by less dangerous, preferably solid sources. Another important aspect is the identification and elimination of intermixing processes other than memory effects, in particular, the intermixing of hetero-epitaxial films at their interfaces due to chemical reactions or diffusion.

In order to identify specific experimental conditions for subsequent studies in space with minimum interference by secondary intermixing effects, we have chosen the system $ZnSi_xGe_{1-x}P_2/GaN_yP_{1-y}/Si$ as a model case. The $ZnSi_xGe_{1-x}P_2/GaN_yP_{1-y}/Si$ heterostructure is of general interest in the context of the integration compound semiconductor and silicon technologies. Also, the system $ZnSi_xGe_{1-x}P_2$ exhibits large birefringence and large nonlinear susceptibility tensor components. It is thus an attractive choice for phase-matched non-linear optical applications, for example, second-and higher-order harmonic generation with CO or CO_2 laser radiation.

RESEARCH APPROACH

As epitaxial techniques, we have chosen remote plasma enhanced chemical vapor epitaxy (RPCVD) and chemical beam epitaxy (CBE) because these methods lend themselves to low temperature processing which minimizes intermixing by diffusion.

Both systems were designed and built by us. The CBE system provides for the controlled injection of four process gases (N_2, H_2, Si_2H_6 and GeH_4) and three organometallic source vapors (t-butyl phosphine, $Ga[C_2H_5]_3$ and $Zn[C_2H_5]_2$). Appropriate safety measures and waste disposal facilities have been incorporated into the system design. Similarly, the RPCVD system has been designed and built by us. Thus far, both systems have performed well and without any emergency incidence. The following research tasks have been completed:

1. The RPCVD of GaN on Si and sapphire substrates using trimethyl gallium and plasma-excited ammonia as source materials.

2. The RPCVD GaP on GaP and Si substrates using trimethyl gallium, hydrogen, and solid phosphorus as source materials.

3. The CBE of GaP on Si using triethyl gallium and t-butyl phosphine as source materials.

4. The organometallic chemical vapor epitaxy of $ZnGeP_2$ and $ZnSi_xGe_xP_2$ on GaP and Si substrates using dimethyl zinc, germane, disilane, and phosphine as source material.

5. The study of the formation of antiphase domains at III-V/IV interfaces; for example, $Al_xGa_{1-x}As$/Ge and GaP/Si interfaces.

6. The characterization of the above heterostructures by electron diffraction, cross-sectional transmission electron microscopy, photoconductivity, photoluminescence, Hall effect measurements, Rutherford backscattering, Auger electron spectroscopy, and secondary ion mass spectrometry. Based on the results of our research, we are currently focusing onto the CBE growth of ZnSiP2 on both GaP and Si substrates and are modifying the RPCVD system for $ZnSi_xGe_{1-x}P$ and GaN_yP_{1-y} growth on GaP and Si substrates, replacing all toxic group V hydride and organometallic compound sources by inorganic solid source materials.

PROGRESS DURING FY1992

Under the conditions of RPCVD, the plasma is physically separated from the location of the substrate: that is, its interactions with the substrate surface by charged particle bombardment are well controlled. The role of the plasma is thus primarily

the in-situ generation of neutral high energy precursor molecules for the vapor deposition process.

For example by injecting phosphorus vapor into a hydrogen plasma, we have been able to replace the need for storing highly toxic and pyrophoric phosphine gas by the utilization of harmless solid red phosphorus and hydrogen/helium gas mixtures, generating phosphine and reactive fragments thereof at the point of use. In addition, the in-situ generation of reactive fragments of phosphine in the hydrogen plasma allows a reduction of the growth temperature as compared to chemical vapor deposition of GaP without a plasma.

Even lower processing temperatures have been achieved with chemical beam epitaxy using liquid organophosphorus sources. However, although the low processing temperature prevents interdiffusion at the interface of Ga and P into the Si and of Si into the GaP at measurable levels, the incorporation of carbon from the organometallic precursors into the GaP film is a problem because the Si/GaP interface represents a perfect sink, where carbon becomes bonded to silicon. Since silicon carbide has a much smaller lattice constant than silicon, this subcutaneous growth of SiC introduces strain at the interface that increases with increasing duration of the growth process, deteriorating both the growth morphology and the perfection of the GaP epilayer. Therefore, current efforts aim at the total elimination of sources of carbon from the growth process. A modification of the RPCVD system that was originally designed for the use of organometallic sources, (OMCVD), is presently underway to accommodate inorganic metal sources. We have already shown that RPCVD can be utilized for the deposition of GaN on Si and sapphire substrates, respectively, and are now focusing onto the growth of GaN_yP_{1-y} films. Also, we have reported the results of a preliminary assessment of the formation of microscopic antiphase domains at defects in the III-V/IV interface, and of the tradeoff between improving interfacial recombination velocity and decreasing bulk life time with decreasing substrate temperature for the well established $Al_xGa_{1-x}As/Ge$ heterostructure.

After demonstrating the feasibility of the heteroepitaxial growth of ZnGeP2 on GaP and Si and of $ZnSi_xGe_{1-x}P_2$ on GaP by OMCVD, current efforts concentrate onto the growth of pure $ZnSiP_2$ on Si and GaP by CBE. Once the conditions for the growth of dilute solid solutions of GaN in GaP are known, we will address the growth of $ZnSi_xGe_{1-x}P_2$ embedded into layers of GaN_yP_{1-y} to investigate confinement and strain effects on the birefringence and phase-matching conditions and other physical properties that are important for device engineering. Also, we have discovered that large concentrations of excess group IV elements can be incorporated into the lattice of $ZnSi_xGe_{1-x}P_2$ under the low-temperature processing conditions developed by us. This provides for continuous bandgap engineering at constant lattice parameter in the pseudo quaternary alloy system Si-Ge-$ZnSiP_2$-$ZnGeP_2$. In particular, the existence of a continuous range of metastable alloys in this system, matching the lattice

constant of silicon exactly, may permit the lattice-matched grading from pure silicon into a $ZnSi_xGe_{1-x}P_2$ epilayer, representing a new approach to the integration of compound semiconductor and silicon technologies.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Bachmann, K. J. Chalcopyrite structure materials. In *A Concise Encyclopedia of Electronic Materials,* S. Mahajan, ed., Oxford: Pergamon Press, Ltd., p. 27, 1992.

— Bachmann, K. J. Lattice-matched heteroepitaxy of wide gap ternary compound semiconductors. In *Wide Gap Semiconductors,* T. Moustakas and J. Pancove, eds., *Mat. Res. Soc. Symp. Proc.* vol. 242, 707 (1992).

— Bachmann, K. J. Wide bandgap semiconductors. Invited paper submitted to *J. Crystal Growth,* 1992.

— Bachmann, K. J., Hwang, H. L., and Schwab, C. *Nonstoichiometry in Semiconductors.* Amsterdam: Elsevier Science Publ., B.V. ,1992.

— Choi, S.W., Bachmann, K. J., Timmons, M. L., Colpitts, T. S., and Posthill, J. B. The growth and characterization of $Al^xGa^{1-x}As/Ge$ heterostructures. *J. Electrochem. Soc.* 139 , 312 (1992).

— Choi, S. W., Lucovsky, G., and Bachmann, K. J. Epitaxial growth of GaP on Si by remote plasma enhanced chemical vapor deposition. Submitted to *J. Vac. Sci. Technol.,* 1992.

— Choi, S. W., Lucovsky, G., and Bachmann, K. J. Remote plasma enhanced chemical vapor deposition of GaP with in-situ generation of phosphine precursors. *J. Vac. Sci. Technol. B10* (3), 1070 (1992).

— Kelliher, J. T., and Bachmann, K. J. Chemical beam epitaxy of GaP on Si using triethylgallium and t-butylphosphine. *Proc. MRS Fall Meeting 1992.,* In preparation, 1992.

— Kelliher, J. T., and Bachmann, K. J. "Chemical beam epitaxy of GaP on Si using triethylgallium and t-butylphosphine." MRS Fall Meeting, Boston, MA, December 1992.

— Bachmann, K. J. "Wide bandgap semiconductors." Invited lecture at the International Summer School on Crystal Growth, Palm Springs, CA August 1992.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Fluid Mechanics and Mass Transfer in Melt Crystal Growth: Macro- and Micro-scale Analysis of Controlled Solidification*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-21-07-07

PRINCIPAL INVESTIGATOR: Dr. Robert A. Brown
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TASK OBJECTIVE/DESCRIPTION

This program is aimed at fundamental understanding of the interactions of heat and mass transfer, melt flow, and interface morphology in the design and interpretation of solidification experiments for growth of crystals on Earth and in space. The ongoing research is a mixture of state-of-the-art computational studies of macroscale transport in large-scale crystal growth systems and of microscale formation of cellular solidification structures. An experimental program for studying mechanisms for microstructure formation in solidification is underway and is supported by theoretical and computational analysis of cellular and dendritic crystal growth of binary alloys.

RESEARCH APPROACH

The research being performed under this program is divided into several distinct tasks according to the application of the research to understanding of either macroscale or microscale features in solidification. These are:

Simulation of Directional Solidification — The application of transient and steady-state calculations of axisymmetric convection in directional solidification systems to the analysis of vertical gradient freeze and Bridgman-Stockbarger configurations for the growth of both semi- conductor and oxide crystals. This project includes development of the simulators, and is to include detailed models for radiative heat transfer and coupling between the temperature, solutal, and convection fields.

Cellular and Dendritic Crystal Growth in Thin-film Solidification — The experimental and computational analysis of the dynamics of cellular interface formation in the thin-film, two-dimensional directional solidification of a binary alloy. The includes the development of a new numerical method for analysis of the transition from shallow to deep cellular surfaces as well as the incorporation of the role of convection on interface morphology into the analysis.

Simulation of Small-scale Floating Zones — The simulation of heat transfer, convection, and interface morphologies in small-scale floating zones. Analysis should predict the onset of instabilities in the zone caused by both surface-tension dimensional convection in directional solidification. This research involves the development of numerical algorithms for solving three-dimensional convection problems with solidification that are robust on medium-grain, parallel processing computers.

Progress During FY1992

The progress to date in each of these projects is summarized in this section:

Simulation of Directional Solidification — The integrated simulation of directional solidification, using the vertical Bridgman configuration, has been expanded to include effects important in the growth of semi-transparent, optoelectronic materials. Most importantly, the simulations now include a band-pass radiation model for the calculation of internal radiation through the crystal, along with a detailed model of heat transfer from the ampoule to the surrounding furnace as well as the calculation of the temperature distribution in the furnace. Simulations have focussed on the calculation of the temperature distribution in BGO crystals grown in this configuration, an important material for gamma ray detection.

Cellular and Dendritic Crystal Growth in Thin-film Solidification — Progress in understanding cellular solidification has come in both theoretical and experimental parts of the program. Using the large-scale, thin-film growth experiment developed under this contract, we have completed a detailed study of the dynamics at the onset of cellular crystal growth (near the onset of morphological instability) for succinonitrile-acetone alloys. These studies show conclusively that no unique wavelength is selected; moreover, the presence of long-time-scale chaotic dynamics is established, in agreement with our previous numerical simulations. Theoretical analysis relying on the presence of co-dimension, bifurcation cell shapes with spatially resonant wavelengths has been used to establish a mechanism for the long-time-scale dynamics. We also have uncovered other mechanisms for interfacial dynamics that are not described by these resonant interactions, and, thus, are not captured by weakly nonlinear analysis.

A finite element simulator for both steady and transient analysis has been developed that includes the effects of thermosolutal convection on the small-scale interface morphology. Initial calculations demonstrate the role of convection as an imperfection in the solute concentration as a catalyst for the onset of morphological instability.

We continue to pursue the development of density functional theory (DFT), based on interatomic interactions, as an approach for describing interfacial phenomena in solidification systems. We have to date developed a very accurate DFT for describing crystal-melt phase equilibria in hardsphere and Lennard-Jones materials.

describing crystal-melt phase equilibria in hardsphere and Lennard-Jones materials. We are now developing a theory for inhomogeneity to describe interfacial regions for these materials.

Simulation of Small-scale Floating Zones — A complete dynamic simulation of axisymmetric convection, heat transfer, and interface morphologies in small-scale, floating-zone systems has been developed for solidification of binary alloys. This simulation is being extended to the analysis of the stability of these steady-state flows (to nonaxisymmetric disturbances) to look for the onset of the traveling wave states caused by surface-tension-driven convection.

Three-dimensional Convection in Solidification — The finite-element/Newton method developed by this research group for solving coupled convection/solidification problems is being adapted for use on medium-grain, parallel computers. Our first calculations are on an Intel i860 hypercube with 32-vector computational elements. We have completed development of an automatic, nested-dissection, domain-decomposition method for the parallel solution of large sets of algebraic equations with finite-element structures. This algorithm is among the fastest available anywhere for this application, and it will be the basis for a very robust resolution of any transport problem using MIMD parallel computers.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Bennett, M. J., Tsiveriotis, K., and Brown, R. A. Nonlinear dynamics in periodically repeated sets of directional solidification cells. *Physical Review B.* 45, 9562–9575 (1992).

— Brown, R. A. Crystal growing systems. Invited paper at NATO Meeting on Interactive Dynamics in Convection and Solidification, Chamonix, France, March, 1992.

— Brown, R. A., Lee, R. C. J., and Tsiveriotis, K. Nonlinear dynamics near the onset of cellular growth during thin-film solidification of a binary allow. On the observability of weakly nonlinear states. *Interactive Dynamics of Convection and Solidification*, Kluwer. S. H. Davis et. al., eds., Amsterdam, pp. 69–72, 1992.

— Kim, D-H., and Brown, R. A. Modeling of transients in growth of HgCdTe by the vertical Bridgman technique. *J. Crystal Growth*, 114, 411–434 (1991).

— Kyrilidis, A., and Brown, R. A. "Ability of nonperturbative density functional theories to stabilize arbitrary solids." American Institute of Chemical Engineers, Los Angeles, November, 1991.

— Kyrilidis, A., and Brown, R. A. Density-functional thermodynamic perturbation theory of Lennard-Jones solids. In Computational Methods in Materials Science, Vol. 278. J. E. Mark, M. E. Glicksman, and S. P. Marsh, eds. Materials Research Society,, 21–26, 1992.

— Kyrilidis, A., and Brown, R. A. Local thermodynamic mapping for effective liquid density-functional theory. *Physical Review A*, 45, 5654–5659 (1992).

— Kyrilidis, A., and Brown, R. A. On the ability of nonperturbative density functional theories to stabilize arbitrary solids. *Physical Review A*, 44, 8141–8181 (1991).

— Lee, J. T. C., and Brown, R. A. "Spatiotemporal chaos near the onset of cellular growth during thin-film solidification of a binary allow." NATO Meeting on Interactive Dynamics in Convection and Solidification, Chamonix, France, March, 1992.

— Lee, C. T., Tsiveriotis, K., and Brown, R. A. Spatiotemporal chaos near the onset of cellular growth in thin-film directional solidification. *J. Crystal Growth*, 121, 536–542 (1992).

— Mehrabi, R., and Brown, R. A. Nonlinear analysis of morphlogical interactions between flow and interface shape in the directional solidification of a binary alloy. Interactive Dynamics in Convection and Solidification, Kluwer. S. H. Davis et. al., eds. Amsterdam, pp. 65–67, 1992.

— Mehrabi, R., and Brown, R. A. "Nonlinear analysis of morphological interactions between flow and interface shape." NATO Meeting on Interactive Dynamics in Convection and solidification, Chamonix, France, March, 1992.

— Tsiveriotis, K, and Brown, R. A. Boundary conforming mapping applied to computations of cellular solidification. *Inter. J. Numer. Meths. Fluids*, 14, 981–1003, 1992.

— Tsiveriotis, K., and Brown, R. A. "The role of codimension-two bifurcation in cellular pattern formation in directional solidification." American Institute of Chemical Engineers, Los Angeles, November, 1991.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Modeling Internal Radiative Transport in Crystal Growth Processes*
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** 674-21-06-07

PRINCIPAL INVESTIGATOR: Dr. Jeffrey J. Derby
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TASK OBJECTIVE/DESCRIPTION

Radiation energy transfer is an important feature in the high-temperature processes used to produce many optical and semiconductor crystals. The goal of this research program is to understand the effects of internal radiation, that is, radiation within a participating medium, in several crystal growth systems of technological importance.

RESEARCH APPROACH

We develop and employ finite element methods to accurately predict radiation transfer in semitransparent media for the complicated, multidimensional geometries of crystal growth systems. These methods are extremely accurate and robust and are applicable to systems of any optical thickness. The prediction of radiation transport is combined with previous heat transfer and hydrodynamic analyses of crystal growth to provide quantitative, predictive capabilities for these processes.

PROGRESS DURING FY1992

We have employed Galerkin finite element methods for modeling the vertical Bridgman growth of semitransparent crystals. We identified the strong influence of internal radiation on the shape and position of the melt/crystal interface and the temperature gradients surrounding it.

An important result of our analyses showed that the coupling of internal radiation through the crystal with conduction through the ampoule walls promoted melt/crystal interface shapes which were highly deflected near the ampoule wall. This "radiative interface effect" has been observed, but not adequately understood, in prior experimental systems. The curvature of the melt/crystal interface in these systems is much more pronounced than that observed in the Bridgman growth of opaque crystals, where the interface deflection at the ampoule wall is attributed to

the thermal conductivity mismatch between ampoule and charge. Calculations demonstrated that a flatter overall interface shape could be achieved through optimization of ampoule material properties and furnace temperature profiles.

We are currently developing algorithms which will employ use of massive parallelism to speed our calculations. The primary disadvantage of our current algorithm is the significant computational expense needed for accurate calculations. This feature has limited our attention to the vertical Bridgman system with a semitransparent crystal and an opaque melt, where the relatively simple geometry is exploited in the calculations. We believe that this new methodology will enable further studies of the vertical Bridgman system where the transparency of the melt is considered and will eventually enable the analysis of the more complicated Czochralski crystal growth system.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Brandon, S. "Analysis of the Bridgman growth of semitransparent crystals." ICCG-10, The Tenth International Conference on Crystal Growth, San Diego, CA, August 16–21, 1992.

— Brandon, S. and Derby, J. J. Finite element methods for analysis of internal radiative heat transfer and solidification in a finite cylindrical enclosure. *Int. J. Numer. Meth. Heat & Fluid Flow 2,* (1992).

— Brandon, S. and Derby, J. J. Heat transfer in vertical Bridgman growth of oxides: Effects of conduction, convection, and internal radiation. *J. Crystal Growth 121*, 473–494 (1992).

— Derby, J. J. "Convection effects in the growth of single crystals." ISSCG-8, The Eighth International Summer School on Crystal Growth, Palm Springs, CA, August 9–15, 1992.

— Derby, J. J. "Finite element methods for CFD in chemical engineering: materials processing applications." US-Japan Symposium on Finite Element Methods in Large-Scale Computational Fluid Dynamics, Minnesota Supercomputer Institute and Army High Performance Computing Research Center, Minneapolis, MN, October 12–14, 1992.

— Derby, J. J. An overview of convection during the growth of single crystals from the melt. Proceedings of the *Eighth International Summer School on Crystal Growth,* ISSCG-8, Palm Springs, CA (August 9–15, 1992).

— Derby, J. J., Brandon, S., and Salinger, A. G. On the Rosseland and differential approximations for predicting the buoyant flow of optically thick fluids. *Int. J. Heat Mass Transfer*. In preparation, 1992.

— Derby, J. J., Brandon, S., Salinger, A. G., and Xiao, Q. Large-scale numerical analysis of materials processing systems: High-temperature crystal growth and molten glass flows. *Comp. Meth. Appl. Mech. Eng.* Submitted 1992.

— Kuppurao, S., and Derby, J. J. Finite element formulations for accurate calculation of radiant heat transfer in diffuse-grey enclosures. *AIChE Journal.* Submitted 1992.

— Salinger, A. G., and Brandon, S. "On the effects of internal radiation on convective flows in high-temperature materials processing systems." Poster, ICCG-10, The Tenth International Conference on Crystal Growth, San Diego, CA, August 16–21, 1992.

— Salinger, A. G., Brandon, S., and Derby, J. J. Steady-state flow transitions in the radiative Rayleigh-Benard problem: Visualizing a bifurcation diagram. *Intern. Video J. Eng. Res.* Submitted 1992.

— Salinger, A. G., Brandon, S., and Xiao, Q. "Computer-aided analyses of high-temperature crystal growth processes." American Institute for Chemical Engineering Summer National Meeting, Minneapolis, MN, August 9–15, 1992.

— Salinger, A. G., Brandon, S., Aris, R., and Derby, J. J. Buoyancy-driven flows of a radiatively participating fluid in a vertical cylinder heated from below. *Proc. Roy. Soc. London A.* Submitted 1992.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Growth of Nonlinear Optical Crystals by Melt Processes*
RESPONSIBLE CENTER: MSFC PROJECT IDENTIFICATION: 674-21-08-13

PRINCIPAL INVESTIGATOR: Dr. Donald O. Frazier
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National Aeronautics and Space Administration
Marshall Space Flight Center, AL 35812
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TASK OBJECTIVE/DESCRIPTION

One major goal of this program is to grow high-quality single crystals and composites of nonlinear optical organic and polymeric materials by the Bridgman-Stockberger process. This may include float-zone and liquid-encapsulated float-zone methods. Organic materials are of interest for use in all optical communication and signal processing systems.

RESEARCH APPROACH

The approach is to study Bridgman-Stockberger, and where desirable, liquid-encapsulated Bridgman-Stockberger organic crystal growth from the melt. Additional focus is on methods for exploiting expected low-gravity-processing advantages of increased stability of low-surface- tension melt zones and reduced convective flows for float-zone crystal growth.

Although organics are desirable for use in optoelectronic devices, their use is hindered by the fragility of organic single crystals. There have been demonstrations that the strength of organics can be improved by aligning the photonic component in a polymer matrix. Bulk composites of aligned nonlinear optical organic crystals in low-molecular-weight transparent polymers having improved mechanical strength and fewer defects might be prepared by growing these composite materials in microgravity by directional solidification. Ground-based research in this area includes identifying mixtures appropriate for developing such composites.

PROGRESS DURING FY1992

A team of researchers with a broad range of disciplines suitable for performing the critical functions in this program is in place in the Chemistry and Polymeric Materials Branch. The team has developed a method for calculating static second- and third-order molecular polarizabilities for screening from a very large variety of possibilities. This same group has made significant progress in the use of molecular mechanics to yield information concerning the orientation of molecules within a given film, crystal, or composite, thus allowing for estimations of second- and

third-order nonlinear coefficients for materials. These methods not only provide good predictive tools, but also allow a critical link between fundamental theory and microgravity processing where defect-free crystals, films, and composites may approach theoretical limits predicted for these optical materials.

There has been significant progress toward the development of melt composites having third-order nonlinear optical properties. Polymethylmethscrylate (PMMA) doped with benzil, the photonic component, shows a dramatic electrooptic effect. Other work on composites shows nonlinear behavior, such as frequency doubling, by PMMA doped with m-nitroaniline. Several pure single crystals have been grown, by directional solidification, with varying degrees of hardness. Hardness, an important property of these materials that puts them at a disadvantage, is estimable by the molecular mechanics method, and will add to the screening and theoretical components of the program.

There is further progress in crystal-polishing technology. Several university relationships have been established in this program. Among them, a joint ventures (JOVE) relationship which has established crystal-polishing technology unique to organics. Other relationships, in crystal characterization, theory, and synthesis are in place with historically Black colleges and universities (HBCUs), other JOVE participants, and traditional universities. A number of significant publications have resulted from these interactions.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Aggarwal, M. D., Wang, W. S., Shields, A. W., Penn, B. G., and Frazier, D. O. A versatile low-cost Czochralski crystal growth system for nonlinear optical organic materials. *Rev. Sci. Instrum, 83* (11), 5451–5482 (1992).

— Penn, B. G., Cardelino, B. H., Moore, C. E., Shields, A. W., and Frazier, D. O. Growth of bulk single crystals of organic materials for nonlinear optical devices: An overview. *Prog. Crystal Growth and Charact. 22*, 19–51 (1991).

— Vankateswarfu, P., He., K. X., Bryant, W., Hyde, H. W., Penn, B. G., and Frazier, D. O. New organic materials for nonlinear optics: Study of highly efficient second harmonic generation from N-Alkyl and N, N-Dialkl derivatives of 4-methyl-8-nitro-2-quinolinamines. *Nonlinear Optical Materials*, 145 (1992).

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Growth of Nonlinear Optical Thin Films/Vapor Processes*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-21-08-12

PRINCIPAL INVESTIGATOR: Dr. Donald O. Frazier
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TASK OBJECTIVE/DESCRIPTION

One major goal of this program is to grow high-quality thin films and single crystals of nonlinear optical organic and polymeric materials by vapor transport processes. Organic materials are of interest for use in all optical communication and signal-processing systems.

RESEARCH APPROACH

The approach is to concentrate on exploiting low-gravity processing following a thorough ground-based research program. The ground-based program will provide a basis for the design and analysis of space-based experiments, and determine growth condition and property relationships needed to grow high-quality thin films and single crystals, reproducibly and in quantity. For thin-film preparation it is important to determine the best substrate to optimize film homogeneity and orientation in unit- and low-gravity environments.

PROGRESS DURING FY1992

A team of researchers with a broad range of disciplines suitable to perform the critical functions in this program is in place in the Chemistry and Polymeric Materials Branch. The team has developed a method for calculating static second- and third-order molecular polarizabilities for screening from a very large variety of possibilities. This same group has made significant progress in the use of molecular mechanics to yield information concerning the orientation of molecules within a given film, crystal, or composite, thus allowing for estimation of second and third-order nonlinear coefficients for materials. These methods not only provide good predictive tools, but also allow a critical link between fundamental theory and microgravity processing, where defect-free crystals, films, and composites may approach theoretical limits predicted for these optical materials.

One particularly interesting class of compounds is polydiscetylenes, which are both crystalline and polymeric. Because of their high conjugated electronic structures, polydiscetylenes are among the best nonlinear optical (NLO) materials known. We

have been actively involved in the design, synthesis, and thin-film growth of polydiscetylenes for both second- and third-order NLO applications. We have synthesized a new nitroaniline with a discetylene function which shows excellent promise as a vapor-deposited film having NLO applications. Some direct evidence for the effects of microgravity growth on thin films already exists for another class of polymers known as phthalocyanines; films grown in microgravity exhibited different polymorphic forms than ones grown on Earth. Efforts on this task have begun to duplicate and extend the work in the phthalocyanines.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

— Palsy, M. S., Frazier, D. O., Abdeldsyem, H., McManus, S. P., and Zaulauf, S. E. Synthesis, vapor growth, polmerization, and characterization of thin films of novel discetylene derivatives of pyrrole: The use of computer modeling to predict chemical and optical properties of these discetylenes and polydiscetylenes. *J. Am. Chem. Soc. 114*, 3247–3251 (1992).

— Penn, B. G., Cardelino, B. H., Moore, C. E., Shields, A. W., and Frazier, D. O. Growth of bulk single crystals of organic materials for nonlinear optical devices: An overview. *Prog. Crystal Growth and Charact. 22*, 19–51 (1991).

— Vankateswarfu, P., He., K. X., Bryant, W., Hyde, H. W., Penn, B. G., and Frazier, D. O. New organic materials for nonlinear optics: Study of highly efficient second harmonic generation from N-Alkyl and N, N-Dialkl derivatives of 4-methyl-8-nitro-2-quinolinamines. *Nonlinear Optical Materials, 145* (1992).

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Electronic Materials*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-21-05-02

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TASK OBJECTIVE/DESCRIPTION

The objectives of this task include improving the understanding and control of crystal growth as it is influenced by gravity.

RESEARCH APPROACH

The approach is to use a coordinated program of modeling, development of diagnostic tools, and experiments.

PROGRESS DURING FY1992

Formulation of semitransparent thermal radiation equations applicable to a wide range of optical semiconductor materials has been done. An interface code was developed to enable the interactive computation of transport processes during solidification, together with the dislocation density map in the growing crystal. The addition of magnetic field interaction with the flow field in conductive melts via the Lorenz force is now standard in our general three-dimensional formulation.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Gokoglu, S., Kuczmarski, M., Veitch, L., Tsui, P., and Chait, A. A numerical and experimental analysis of reactor performance and deposition rates for CVD on monofilaments. *Proceedings of the 11th Int'l. CVD Conf., Seattle, 1990*. The ElectroChemical Society, 1992.

— Peltier, L. J., Biringen, S., and Chait, A. Application of implicit numerical techniques to the solution of the three-dimensional diffusion equation. *J. Numerical Heat Transfer,* in preparation, 1992.

— Young, G. W., and Chait, A. Steady-state thermal solutal diffusion and convection in a float-zone. In *Progress in Low-Gravity Fluid Dynamics and Transport Phenomena.* J. N. Koster and R. L. Sani, eds. AIAA 1990. In preparation, 1992.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Microgravity Materials Science Laboratory*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-21-05-01

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TASK OBJECTIVE/DESCRIPTION

The Microgravity Materials Science Laboratory (MMSL) laboratory was established to provide to researchers from industry, academia, and the government access to specialized equipment and experienced personnel, to aid in the development of space flight concepts, experiments, and hardware. The laboratory is equipped with a number of unusual experimental and computational facilities; it is staffed by engineers from several disciplines and by technicians who are familiar with microgravity practices.

RESEARCH APPROACH

In the MMSL, investigators are encouraged to take the first step toward defining space flight experiments for later performance on the Space Shuttle or on Space Stations Freedom. The MMSL may also be used in preparation for experiments to be conducted in other ground-based, reduced-gravity environments such as those provided by drop-tubes, aircraft, or rockets. The computational facilities may be used to model the expected fluid-flow and heat transfer in microgravity experiments. Another use of the laboratory is for postflight investigations.

PROGRESS DURING FY1992

MMSL was used primarily by Lewis researchers, although cooperative projects have been performed with Westinghouse, GTE, Marshall Space Flight Center (MSFC), Case Western Reserve University (CWRU), Cleveland State University (CSU), University of Colorado, Texas Instruments, University of Toledo, Ohio State University, and the Space Experiments Division. The MMSL provides facilities for the Programmable Multi-Zone Furnace (PMZF) project, the Advanced Furnace Technology ATD project, the Laser Light Scattering ATD project, and the Surface Light Scattering Instrument ATD project.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Arnold, W. A., Jacqmin, D. A., Gaug, R. L., and Chait, A. Flow phenomena in directional solidification during space processing: Two-vs. three-dimensional transport modes. In preparation, *AIAA J. of Spacecraft and Rockets,* 1992.

— Arnold, W. A., Wilcox, W. R., Carlson, F., Chait, A., and Regal, L. Transport model during crystal growth in a centrifuge. *J. of Crystal Growth, 119,* 1992.

— Auping, J. V., and Johnston, J. C. Modula-2 from a new user's perspective. *Dr. Dobbs' Journal.* In preparation, *AIAA J. of Spacecraft and Rockets,* 1992.

— Chait, A., Johnston, C., Thompson, D., and Glasgow, T. Modeling materials experiments: Lewis at forefront of emerging science. *NASA TechBriefs,* 15, 10, October 1991.

— Chiaramonte, P. P., Foerster, G., Gotti, D. J., Neumann, E. S., and Johnston, J. C. Initial study of void formation during aluminum solidification in reduced gravity. *J. of Spacecraft and Rockets, 29,* 5, (October 1992).

— de Grob III, H. C., and Kassemi, M. Effect of radiation on convection at moderate temperature. Submitted to ATAA *J. of Thermophysics and Heat Transfer,* 1992.

— Hahn, R. C., Johnston, J. C., Herbach, B. A., and Bethea, M. Determinationof the critical parameters for remote microscope control. *Microgravity Quarterly* 2, 1, (1992).

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— Raz, E., and Chait, A. Velocity and morphology transition in dendritic growth. *MRS SOC.* ser. 237199, 1992.

— Raz, E., Lipson, S. G., and Ben-Jacob, E. New periodic dendritic morphologies observed during dendritic growth of ammonium chloride crystals grown in thin layers, *J. of Crystal Growth,* vol. 10, no. 8, 1991, pp 637–646.

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TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Growth of Organic Single Crystals by Two Modified Floating-Zone Processes*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-21-07-09

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TASK OBJECTIVE/DESCRIPTION

This is a 1-year project with the goal of growing organic single crystals by a floating-zone-type technique. Organic single crystals have been used for scintillation and nonlinear optical materials. As compared to the Bridgman and Czochralski techniques, the advantages of the floating-zone-type technique are (a) no mechanical damage induced by the ampoule, and (b) minimum chemical degradation due to prolonged heating of the melt. Unfortunately, the surface tension of organic melts is too low to allow floating-zone growth under normal gravity—the melt zone collapses and crystal growth is disrupted. Under microgravity, however, zone instability is no longer a problem. The objective of this project is to learn how to first grow organic single crystals by floating-zone-technique on the ground. The information gathered can be used to help design future flight experiments.

RESEARCH APPROACH

Two modified floating-zone processes, developed in our previous NASA study and patented recently, have been adopted. These two processes are unique in that a shaper is used to (a) define the cross-section of the melt and hence the growing crystal and (b) suppress undesirable oscillatory thermocapillary convection in the melt. In modified process (a) the shaper is in the form of a ring covering most of the melt surface, whereas in modified process (b) it is in the form of a disk immersed in the melt zone.

PROGRESS DURING FY1992

Organic single crystals have been grown by floating-zone process for the first time. Benzil crystals were grown about 6 mm in diameter, 8 cm long, and with a very uniform cross-section. Salol crystals were grown up to about 10 cm long, including rectangular crystals about 9 mm x 3 mm in cross section.

These crystals were grown with the help of round and rectangular aluminum shapers, which are chemically compatible with the melts of both organic materials.

The aluminum shapers were carefully kept at a constant temperature just above the melting points of the organic materials, with a thermocouple, a resistance heater, and a temperature controller. These results suggest that the two modified processes can be very useful for future growth of larger organic single crystals in space.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kou, S., and Chen, C. P. Modified floating-zone growth of organic single crystals. Manuscript in preparation, 1992.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Process Modeling for Materials Preparation*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-21-08-08

PRINCIPAL INVESTIGATOR: Prof. Franz Rosenberger
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TASK OBJECTIVE/DESCRIPTION

The objectives of this program are the exploitation and improvement of available numerical techniques to formulate and solve useful models of transport processes in (microgravity) materials preparation experiments. This capability will lead to the efficient design of materials processing experiments for optimal use of the limited opportunity and duration of microgravity flight experiments.

RESEARCH APPROACH

The potential of the most sophisticated modeling techniques can only be fully realized if the physical properties, boundary conditions, and operating conditions are well characterized. Recognizing this, we are conducting a comprehensive research program that coordinates a study of transport properties with the development of numerical models for two specific crystal growth systems:

1. Growth of mercury cadmium telluride (MCT) from the melt by the Bridgman-Stockbarger technique; and

2. Growth of triglycine sulfate (TGS) from solution.

The transport property studies, made under temperature and supersaturation conditions representative for processing, include (a) kinematic viscosity measurements of molten MCT at temperatures close to the composition dependent melting, (measurements are made for different compostions); and (b) solute diffusivity measurements in aqueous TGS solutions. The numerical modeling studies include the development of an algorithm which employs Chebyshev spectral techniques to solve a moving boundary problem; incorporation of this technique into a pseudospectral collocation method that we have previously applied to convective-diffusive transport in melts; and development of numerical methods for the specific moving boundary problems associated with the growth of MCT by the Bridgman-Stockbarger technique.

PROGRESS DURING FY1992

We have developed a novel version of the capillary method for kinematic viscosity measurements. Viscosity data can be deduced in a straightforward way from mass transfer data obtained by differential weighing during gravity-driven flow of the liquid between two cylindrical chambers. The technique facilitates operation under sealed, isothermal conditions and thus is particularly well suited for high-temperature and high-pressure liquids. For melts with high surface tension, however, it is difficult to drive flow through small capillaries with small hydraulic heads. Hence, we have resorted to the oscillating-cup viscometry technique for studies of molten MCT. For the viscosity of MCT of composition $Hg_{.79}Cd_{.21}Te$ at 795 °C (Tliquidus = 790 °C) we have obtained m = 2.5 ± 0.3 cp. Furthermore, we have completed the development of a novel interferometric technique for the determination of solute diffusivities from the evolution of the concentration profile between two solutions of slightly different concentration. Though similar to the widely used Gouy technique, our approach requires neither an initially sharp boundary between the solutions, nor the assumption of a constant diffusivity. In addition, this approach allows for diffusivity measurements over a range of temperatures in a single experiment. This was not possible with earlier methods. This last feature is particularly important for an efficient conduct of space experiments. The technique has been thoroughly tested with highly concentrated NaCl solutions. The results for undersaturated solutions compare favorably with published values. For supersaturated solutions, however, significantly lower values were obtained than reported by others. We are currently applying the technique to TGS solutions.

A pseudospectral method for (axisymmetric) directional solidification problems has been developed, tested, and applied to a variety of different solidification situations. The method combines domain decomposition with a preconditioned generalized conjugate residual (PGCR) method together with a Picard-type iterative scheme to solve the steady momentum, mass, and heat transfer equations along with the location of the crystal-melt interface. The computational space is decomposed into domains that correspond to the melt, crystal, and ampoule. Since the shape of the melt-crystal boundary is unknown, these domains generally have an irregular shape. The governing equations are mapped from these irregularly shaped domains onto rectangular domains. The resulting equations are then solved iteratively using a PGCR scheme suitable for nonsymmetric systems. We are currently investigating the influence of dopant transport on interface shape. Besides the moving boundary problem, we have developed a pseudospectral Chebyshev collocation method for 3-D convection (without solidification) in a cylinder. Flow transitions (and the consequences for dopant transport) in a simplified (2D Cartesian) model of Bridgman-Stockbarger crystal growth have also been studied.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Alexander, J. I. D. "Modeling or muddling? Analysis of buoyancy effects on transport under low gravity conditions." Invited lecture, World Space Congress, Washington DC August 28–September 5, 1992.

— Alexander, J. I. D. "Numerical simulation of low-g fluid transport." Lecture, AIAA course on low-gravity fluid mechanics. Reno, NV, January 10–12, 1992.

— Alexander, J. I. D. "Vibrational convection and transport under low-gravity conditions." Society of Engineering Science, 28th Annual Technical Meeting, Gainesville, FL, November 6–7, 1991.

— Larroude, P., Ouazzani, J., and Alexander, J. I. D. "Flow transitions in a 2D directional solidification model." Poster, 6th Materials Science Symposium, European Space Agency, Brussels, Belgium, 1992.

— Larroude, P., Ouazzani, J., and Alexander, J. I. D. Symmetry breaking flow transitions and oscillatory flows in a 2D directional solidification model. Accepted for*European Journal of Mechanics*,, 1992.

— Nadarajah, A. "Modeling crystal growth under low gravity." Society of Engineering Science, 28th Annual Technical Meeting, Gainesville, FL, November 6–7, 1991.

— Nadarajah, A., and Rosenberger, F. Integral method for diffusivity measurements in liquids, *J. Phys. Chem.* Submitted 1992.

— Pulicani, J. P., and Ouazzani, J. A Fourier-Chebyshev pseudospectral method for solving steady 3-D Navier-Stokes and heat equations in cylindrical cavities. *Computers Fluids 20* 93–109 (1991).

— Pulicani, J. P., Krukowski, S., Alexander, J. I. D., Ouazzani, J. and Rosenberger, F. Convection in an asymmetrically heated cylinder, *Int. J. Heat Mass Transfer 35* 2119-2130 (1992).

— Rosenberger, F. Boundary layers in crystal growth, facts and fancy. *In Lectures on Crystal Growth* (H. Komatsu, ed.).

— Rosenberger, F. "Computer simulation in materials science." Invited lecture, Mitsubishi Frontiers Research Institute, Tokyo, Japan, November 8, 1991.

— Rosenberger, F. "Importance of materials research in space laboratories for industrial development." Plenary lecture, International Symposium for Promoting Applications and Capabilities of the Space Environment, Tokyo, Japan, November 14–15, 1991.

— Rosenberger, F. "Microgravity materials processing and fluid transport." Lectures, AIAA course on Low-Gravity Fluid Dynamics. Reno, NV, January 10–12, 1992.

— Rosenberger, F. "Theoretical review of crystal growth in space - motivation and results." Plenary lecture, International Symposium on High Tech Materials, Nagoya, Japan, November 6–9, 1991.

— Rosenberger, F. "Time scales in transport processes and challenges for short-duration low-gravity experiments." Invited lecture, Falltower Days Bremen, Bremen, Germany, June 1–3, 1992.

— Rosenberger, F. "What can one learn from 10 second low-gravity Experiments?" Plenary lecture, In Space 1991, Tokyo, Japan, November 14–15, 1991.

— Rosenberger, F., Alexander, J. I. D., and Jin, W.-Q. Gravimetric capillary method for kinematic viscosity measurements. *Rev. Sci. Instruments 63* 4196-4199 (1992).

— Zhang, Y., Alexander, J. I. D., and Ouazzani, J. A Chebyshev collocation method for heat transfer, interface shape and convection during directional solidification. *International Journal of Numerical Methods in Heat and Fluid Flow.* To be published 1993.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Theory of Materials Growth in Space: The Liquid-Solid Interface*
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** 674-21-06-08

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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to advance the theory of microgravity crystal growth through accurate models of the phenomena occurring at the liquid-solid interface and their influence on the crystal perfection ultimately produced. To accomplish this objective with accuracy, we had to refine several of our computational tools and develop some new ones. The principal advances required are these:

1. Refine and compound our alloy Hamiltonian for inclusion in our surface Green's function calculation of the interactions among surface atoms and their sublimation energies. This establishes the parameters needed to set the surface order-disorder state and the growth rate.

2. Add effects that are due to having a liquid-solid interface rather than the vacuum-solid interface we treated previously by first modeling the liquid as a homogeneous dielectric medium and then refining the liquid model to include structure factors, configurational entropy, and excitation entropy terms.

3. Relate the interface properties to the final bulk crystal properties (short-range order state, native defect densities, etc.) through an appropriate statistical theory, for various sets of external control parameters.

RESEARCH APPROACH

We propose to begin with a reliable and accurate band structure, based on first principles, that can treat surfaces and other situations where there are large distortions. The interaction energies between the constituent atoms, in an alloy, are then obtained by employing coherent potential approximation (CPA) energies in a generalized perturbation method (GPM). At low temperatures, the phase diagram can be determined from these interaction energies. For compounds, however, the pair energies are deduced, as before, from sublimation energies calculated from these accurate band structures.

From the combined knowledge of sublimation and pair energies, we can calculate the growth rate from a Boltzmann-type equation. The main impact of this work is in the treatment of growth for external control-parameter sets where equilibrium is not reached for all processes; for example, some native defect concentrations.

PROGRESS DURING FY1992

We now have established first principles based on self-consistent Hamiltonian in a tight-binding form from which we can generate accurate band structures and structural properties such as total energies, bulk moduli, and equilibrium lattice constants. With addition of d-orbitals and an ad hoc site diagonal potential, we can obtain the lowest conduction band in good agreement with experiment. The finite nature of the basis set (four to nine orbitals per atom), has precluded more rigorous methods, such as GW approximation, to correct the gap. Because the surface states are derived from both conduction and valence bands edge properties we have focused on near-gap band structures.

We generalized our existing Green's function method for nonorthogonal bases with interactions extending beyond second neighbors. The corresponding CPA and GPM are also generalized to suit. As a test, we applied this procedure to GaAlAs. Its excess energy, which is near zero in the bulk alloy, reduces dramatically on (100) surfaces, giving rise to Cu-Au ordering at lower temperatures with a critical temperature of about 900 K. Such an ordering was observed in 1985, and our calculation is the first to successfully explain this observation. We also use generalized Green's functions to obtain surface orientation and coverage-dependent sublimation energies. These energies and excess pair energies will be used to study crystal growth rates. These accomplishments satisfy the first advance needed to reach our stated objective.

While we worked primarily on developing computational techniques for the surface and interface energetics needed for growth modeling, we also reviewed state-of-the-art phase-diagram calculations and data. Although the structures of semiconductors and their alloys in the liquid phase are inherently complex, the simple regular-solution or quasi-chemical approximation (QCA) has been shown to work very well for GaAs, InAs, and InSb, and for their alloys. For CdTe, HgTe, and PbTe, modifying QCA to include a molecular species (the associate solution model) has been shown to be sufficient. In these models, the data needed are the melting temperatures, entropy difference between the liquid mixture and the ordered solids, the effective coordination number z, and effective pair interactions. These parameters still do not describe the underlying structure of the liquid, which is needed to understand the liquid-solid interface on the microscopic scale; they do however, suggest a model for the liquid.

Stringfellow and Kikuchi found that an effective coordination number, $Z = 6$, works well for the liquid phase. This number, plus the increase in density going from solid to liquid, suggests that liquid is more closely packed. One possible way to

change from the fourfold coordinated zinc-blende (zb) to a closer-packed system is to compare the zb with the CsCl structure. If zb is viewed as an ordered CsCl structure with half of the atoms missing from each sublattice, then the Z=6 liquid may correspond to a disordered and expanded CsCl structure with 1/4 of the atoms missing. The disorder caused by the exchange occupancy of atoms and vacancies (and possibly between cations and anions), softer mode vibrational excitations, and further allowance of more free volume for the atoms in the liquid will raise the entropy as compared with the crystalline solid.

The entropy change from disorder contributions, however, is estimated to be at most 3k per atom, far less than the 7k used in the phase diagram calculation by Stringfellow and Kikuchi.

The balance can be explained if the vibrational mode frequencies in the liquid are four times smaller than those in the solid. They assume that the change of heat capacities in the phase transition is zero, which in general is not the case. Completion of a detailed liquid model will permit us to address these questions and will enable us to calculate the energy parameters and the distribution of host and impurity atoms across the liquid-solid phase boundary.

We have completed a theory of the short-range order state of bulk semiconductor alloys, an essential ingredient in a theory that couples the surface order state to the bulk material state in the temperature gradient behind the growth front.

Thus, we have already built many of the tools needed to determine the liquid- to solid-growth interface state properties and relate them to those of the resulting bulk solid, but still have to exercise these tools and assemble them into a system to meet the objective of this program.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Berding, M. A., Sher, A., and Chen, A.-B. $Hg_{1-x}Cd_xTe$: Defect structure overview. *Mat. Res. Soc. Symp. Proc.*, vol. 216, p. 3 (1991).

— Krishnamurthy, S., Chen, A.-B., and Sher, A. A first principles tight-binding bandstructure method for semiconductors. For *Phys. Rev. B.* In progress, 1992.

— Krishnamurthy, S., Berding, M. A., and Sher, A. Surface energies and order-state: Effects on semiconductor growth. in *Computer Aided Innovation of New Materials*, M. Doyama, T. Suzuki, J. Kihara, and R. Yamamoto, eds. Elsevier Science Publishers B. V., North-Holland, 1992, p. 681.

— Krishnamurthy, S., Chen, A.-B., and Sher, A. Surface-induced ordering of GaAlAs. For *Phys. Rev. Lett.* In progress, 1992.

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— Krishnamurthy, S., Berding, M. A., Sher, A., and Chen, A.-B. Epitaxially grown semiconductor surfaces. *J. Crystal Growth*, vol. 109, (1991) pp. 88–93.

— Krishnamurthy, S., Berding, M. A., Sher, A. and Chen, A.-B. Semicondcuctor surface sublimination energies and atom-atom interactions. *Phys. Rev. Lett.*, vol. 64, no. 21, p. 2531.
— Sher, A., and Chen, A.-B. Alloy statistics and phase diagrams. For *Phys. Rev.* In progress, 1992.
— Sher, A., Berding, M. A., van Schilfgaarde, M., and Chen, A-B. HgCdTe status review with emphasis on correlations, native defects, and diffusion. *Semicond. Sci. Technol. 6,* 1991, C59–C70.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Growth Kinetics of Physical Vapor Transport Properties: Crystal Growth*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-21-05-08

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TASK OBJECTIVE/DESCRIPTION

The objective of this task is to study the relationship between growth parameters during the growth of mercurous chloride by the physical vapor transport (PVT) technique, and diffusive instabilities during the PVT process.

RESEARCH APPROACH

The approach has been to purify and grow mercurous crystals under various conditions in order to deduce relationships between growth parameters and crystal quality.

PROGRESS DURING FY1992

There is an ongoing correlation of crystal-growth velocity with orientation of experiment apparatus, with respect to the the velocity vector. The effect of growth variables on morphology, aspect ratio, and gravity vector were studied; data were correlated with recent theories to evaluate the role of convection; and crystal growth rate is being measured at various vector orientations. Characterization techniques at Westinghouse have been developed to access the quality of grown crystals.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Vapor Crystal Growth of Electro-optical Materials*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-21-08-11

PRINCIPAL INVESTIGATOR: Dr. Frank R. Szofran
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TASK OBJECTIVE/DESCRIPTION

This project is nearly complete. Its goal has been to establish the effects of the processing environment, including gravitational orientation, on the nature and distribution of defects on materials of substantial technological interest that can be grown by the physical vapor transport method. The primary candidate materials were CdS and CdTe.

The investigation was intended to define a flight experiment that would take full advantage of the Vapor Crystal Growth Furnace (CVTE) developed by Boeing Aerospace Company. Two sample positions in that furnace were made available to MSFC on the first flight of the CVTE. The strategy included the development of a 1-g crystal growth data base and extensive characterization of both the starting materials and the grown crystals. A method to simulate reduced gravity has not been devised for this growth method but crystals were grown at different orientations with respect to the gravity vector to assess the effects of gravity on Earth. The material for the first flight was CdTe.

RESEARCH APPROACH

Favorable growth parameters in a laboratory furnace have been established. Work with Boeing was conducted in the Boeing laboratory and ground control furnaces in Seattle. UAH has analyzed both ampoule and sample materials, and results indicate that adequate purity for achieving the project objectives exists in the starting materials and is maintained during the CdTe compounding process. Purity of CdTe crystals following the growth process will be determined.

In addition to CdTe and CdS, high-quality crystals of ZnTe, PbS, and PbSe have been grown in the laboratory at MSFC using the technique developed under this project. The ZnTe crystals grown under this project have optical transmission and photoluminescence spectra that are featureless as opposed to various bands observed in the spectra of ZnTe grown by the traveling heater method (THM).

PROGRESS DURING FY1992

UAH has continued and expanded the impurity analysis work to include atomic absorption detection of lithium, potassium, and sodium in both elemental Cd and Te and compounded CdTe.

Physical vapor transport crystal growth has continued in the Space Science Laboratory.

This ground-based work carried out at MSFC and additional growth runs in the Boeing laboratory were used to improve the growth parameters as much as possible. Nonetheless, more growth runs in the ground control furnace would have been helpful to better define the optimum parameters for the flight experiments.

The CVTE was flown in the mid-deck accommodations rack (MAR) on STS-52. Two furnaces were run sequentially during the mission. Each furnace contained two samples—one for Boeing and one for MSFC. The first MSFC sample was seeded and was intended to be the longer duration growth time. Unfortunately, this furnace was unintentionally shut down early and had a growth time of only 22.73 hours. The second sample was unseeded and, with the additional time available because of the foreshortened first run, had a total growth time of 56.76 hours. The samples are now in Seattle and have not been returned to MSFC at the time this is being written.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Sha, Y.-G., Su, C.-H., Gillies, D. C., Volz, M. P., Lehoczky, S. L., and Szofran, F. R. "Transport rate and epitaxial growth of HgZnTe by chemical vapor transport in a closed ampoule." Presented at the 10th International Conference on Crystal Growth (ICCG-10), San Diego, California, August 16–21, 1992.

— Su, C.-H., Lehoczky, S. L., and Szofran, F. R. An improved vapor growth method for the preparation of electronic and electro-optical materials. *NASA Tech Briefs*. In press, 1992.

— Su, C.-H., Volz, M. P., Gillies, D. C., Szofran, F. R., Lehoczky, S. L., Dudley, M., Yao, G.-D., and Zhou, W. Growth of ZnTe by physical vapor transport and traveling heater method. Presented at the 10th International Conference on Crystal Growth (ICCG-10), San Diego, California, August 16–21, 1992. Accepted *J. Crystal Growth*. 1992.

— Volz, M. P., Su, C.-H., Lehoczky, S. L., and Szofran, F. R. Vibronic spectra of Cu2+ in ZnTe. *Physical Review* B 46 76-82 (1992).

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: ***Modeling Directional Solidification***
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-21-08-10

PRINCIPAL INVESTIGATOR: Dr. William R. Wilcox
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TASK OBJECTIVE/DESCRIPTION

The project objective is to gain an improved understanding of the influence of gravity on the directional solidification of compound semiconductors and their alloys.

RESEARCH APPROACH

Research was designed to determine experimentally:

1. The influence of current pulses, vibration, and accelerated crucible rotation technique (ACRT) on the compositional homogeneity and microstructure of InSb-GaSb alloy;

2. The variation of freezing rate during a spin-up/spin-down cycle by using current pulses during solidification of doped InSb; and

3. The influence of vibration and ACRT on the interface shape of doped InSb using current pulses during solidification.

PROGRESS DURING FY1992

The first task was completed prior to FY 1992. The second was partially completed in FY 1992. The freezing rate varied significantly during each ACRT cycle. The number of striations observed was less than the number of current pulses, indicating that the freezing rate was sometimes very low or even negative. The influence of experimental conditions is being determined.

Progress has been made on the third task. The ACRT and vibration conditions used thus far do make the interface slightly more convex. Additional solidification conditions are being investigated.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Gray, R. T., and Wilcox, W. R. Influence of the accelerated crucible rotation technique on directional solidification of InSb-GaSb slloys. *J. Spacecraft & Rockets* , in press , 1992.

— Gray, R., Banan, M., Zhou, J., Larrousse, M., and Wilcox, W. R. "Influence of perturbations on directional solidification of InSb-GaSb alloy semiconductors." AIAA, Reno, NV, January 1992.

— Neugebauer, G. T., and Wilcox, W. R. Experimental observation of the influence of furnace temperature profile on convection and segregation in the vertical Bridgman crystal growth technique. *Acta Astronautica 25*, 357–362 (1991).

— Zhou, J., Banan, M., Gray, R., and Wilcox, W. R. "ACRT striations and the use of current interface demarcation during directional solidification of Te-doped InSb." Fourth Eastern Regional Conference on Crystal Growth (ACCG/East-4), Atlantic City, NJ, October 1991.

— Zhou, J., Larrousse, M., and Wilcox, W. R. "Directional solidification with ACRT." Tenth International Conference on Crystal Growth (ICCG-10), San Diego, CA, August 1992. In press, *J. Crystal Growth,* 1992.

TYPE: Ground
DISCIPLINE: Electronic Materials
PROJECT TITLE: *Crystal Growth of Device Quality GaAs in Space*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-21-07-06

PRINCIPAL INVESTIGATOR: Dr. August F. Witt
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TASK OBJECTIVE/DESCRIPTION

A heat-pipe-based, vertical growth facility for operation in Bridgman and gradient-freeze modes has been designed, constructed, and put into operation. The hot zone of the system is configured for basic compatibility with NASA's Crystal Growth Experiment Furnace (CGF) hardware.

Growth research was focused on the establishment and characterization of quantifiable thermal boundary conditions in gradient-freeze mode and the achievement of control over initial transients and end effects. The development of new approaches to noninvasive, optical characterization of electronic and opto-electronic materials was extended from GaAs to $Bi_{12}SiO_{20}$ (BSO), a system under consideration for growth and segregation studies in reduced-gravity environment.

RESEARCH APPROACH

Considering the desirability of conducting growth experiments in space on a quantifiable basis to which mathematical modeling is applicable, the achievement of controllable and quantifiable thermal boundary conditions in Bridgman-type configuration, as well as the elimination of extended initial transients and end effects, were primary goals to be addressed.

The stated objectives were approached using heat pipes and a reconfigured temperature control system. Also initiated was research on growth and characterization of bismuth silicate ($B_{12}SiO_{20}$). The Czochralski technique was selected for the growth of seed material, and diversely doped crystals were required for the development of optical approaches to the quantitative characterization of crystalline and chemical defects in this material.

PROGRESS DURING FY1992

Accomplishments in FY92 were as follows:

1. A Bridgman-type growth system with quantifiable and controllable thermal boundary conditions, permitting crystal-melt interface stabilization during growth, has been developed and is being characterized;

2. A Czochralski system for growth of $B_{12}SiO_{20}$ has been placed in operation, and noninvasive optical characterization of this material has been developed, and

3. The program, "Undergraduate Research Opportunities in Microgravity Science and Technology," initiated at MIT within the framework of this proposal, has reached a stage where KC-135 flight experiments are prepared for execution. The experiments are designed to provide a data base for the establishment of nonwetting conditions during crystal growth in a reduced-gravity environment. Systems being investigated include: InSb, GaSb, Ge, GaInSb, $B_{12}SiO_{20}$ and $B_{12}GeO_{20}$.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Cao, X. Z., and Witt, A. F. Identification of dislocation etch pits in n-type GaAs by NIR transmission microscopy. *J. Crystal Growth 114*, 225–257 (1991).
— Carlson, D. J., and Witt, A. F. Quantitative analysis of the effects of vertical magnetic fields on microsegregation in Te-doped LEC GaAs. *J. Crystal Growth 116* (3/4), 461–472 (1992).
— Wargo, M. J., and Witt, A. F. Real time thermal imaging for analysis and control of crystal growth by the Czochralski Technique. *J Crystal Growth 116* (1/2) 213–224 (1992).
— Witt, A. F. "Characterization of GaAs wafers." Intel Corporation, Santa Clara, CA, March 4, 1992.
— Witt, A. F. "Gravitational effects on crystal growth and segregation." 30th Aerospace Sciences Meeting and Exhibit, AIAA, Reno, NV, January 7, 1992.
— Witt, A. F. "New approaches to non-invasive semiconductor characterization." Tenth International Conference on Crystal Growth, San Diego, CA, August 18, 1992.
— Witt, A. F. "Non-invasive wafer characterization." Motorola Corporation, Tempe, AZ, March 6, 1992.

PATENTS — Cao, X. Z., and Witt, A. F. "Apparatus for Accelerated Dislocation Density Mapping. Submitted, MIT Case No. 6126.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***Reactive Fluids Experiment: Chemical Vapor Deposition***
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** 674-24-06-03

PRINCIPAL INVESTIGATOR: Dr. Ivan O. Clark
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TASK OBJECTIVE/DESCRIPTION

The research will develop a series of ground-based experimental investigations of the fluid dynamics of chemical vapor deposition (CVD) which will lead to an enhanced understanding of the basic sciences underlying reactive fluid interactions. It will form the basis for a proposal to perform a series of flight experiments necessary to more fully elucidate these scientific principles. This program will use past experience in chemical vapor deposition, nonisothermal flow measurements, numerical modeling of reactive fluid dynamics, and development of instrumentation to carry out the research.

RESEARCH APPROACH

A combined numerical and experimental approach is being used to investigate the CVD process. The experimental approach combines growth of semiconductor materials, the deposition of a model material, and the measurement of the gas flow velocities in the CVD reactor using laser velocimetry. The numerical approach models each of the experimental approaches and uses the experimental results for validation.

PROGRESS DURING FY1992

The numerical modeling of InP has been extended to three spatial dimensions with good initial results. The model has proven to be very sensitive to temperature distributions on the CVD reactor walls.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Black, L. R., Clark, I. O., Kui, J., and Jesser, W. A. 3-D numerical modeling of InP MOCVD with comparison to growth experiments. *Proceedings of the Fluent Inc. 1992 Users' Group Meeting*, Burlington, VT, October 13–15, 1992.

— Black, L. R., Clark, I. O., Kui, J., and Jesser, W. A. "3-D Numerical modeling of InP MOCVD with comparison to growth experiments." *Fluent Inc. 1992 Users' Group Meeting,* October 13–15, 1992, Burlington, VT, (1992).

— Clark, I. O., Gerdes, W. K., Black, L. R., Jesser, W. A., Kui, J., Johnson, E. J., Hyer, P. V., and Culotta, P. W. Gravitational and thermal effects in CVD flow and deposition. AIAA 30th Aerospace Sciences Meeting, January 6–9, 1992, Reno, NV. *Proceedings of AIAA 30th Aerospace Sciences Meeting,* Reno, NV January 6–9, 1992, AIAA Paper No. 92-0602, (1992).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Fluid Interface Behavior Under Low-and Reduced-Gravity Conditions*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-28

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TASK OBJECTIVE/DESCRIPTION

The objective of this investigation is to develop a better understanding of the physical behavior of fluids in partly filled containers in low-gravity environments.

RESEARCH APPROACH

The approach for this research task is to pursue parallel theoretical, computational, and experimental studies to examine the fluid surface shape for a variety of vessel/fluid combinations when capillary forces dominate. The studies deal principally with the physical validity of the concept of contact angle as envisioned by the classical Young-Gauss theory, and with unique vessel/fluid conditions for which there are no available theoretical abilities to predict the surface shape.

PROGRESS DURING FY1992

The emphasis of the FY1992 efforts was on the conduct of the Interface Configuration Experiment (ICE) which flew aboard the USML-1 mission as a Glovebox experiment in June 1992. The experimental approach was simply to observe the liquid or vapor surface at equilibrium in a reduced-gravity environment.

Unique in this experiment is the particular shape of the container. The rotational symmetric shape was determined numerically and has the intriguing property that for a given fluid and fill level, an infinite number of rotationally symmetric surfaces (a continuum) exists of identical mechanical energy. As a result, no such surface is preferred, as all have an equal likelihood of forming in lowgravity. A mathematical proof was developed which revealed that nonasymmetric perturbations produce surface shapes of lower energy; meaning, in low-gravity, an asymmetric surface is most likely to be present.

This is indeed what was observed during the flight experiments. In fact, though preliminary numerical solutions revealed a number of lower-energy asymmetric

shapes, only one was established on orbit. Disturbances to this configuration by the payload specialist proved this asymmetric surface shape to be surprisingly stable. Analysis of the data is in progress and was first reported in Reno, January 1993, at the AIAA conference.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Concus, P. Aerospace Engineering Colloquium, University of Milan, Italy, October 1991.

— Concus, P. Applied Mathematics Colloquium, Arizona State University, April 1992.

— Concus, P. First International Congress on Nonlinear Analysis, Tampa, FL, August 1992.

— Concus, P. International Conference on Nonlinear Partial Differential Equations, Plovdiv, Bulgaria, August 1992.

— Concus, P. International Symposium on Motion by Mean Curvature, Povo, Italy, July 1992.

— Concus, P., and Finn, R. On accurate determination of contact angle. *Microgravity Science and Technology*, IV pp. 69–70 (1991).

— Concus, P., and Finn, R. Capillary surfaces in exotic containers. *In Hydromechanics and Heat/Mass Transfer in Microgravity*, V. S. Avduevsky, et al,, eds. London: Gordon and Breach, 1992, pp. 193–196.

— Concus, P., Finn, R., and Weislogel, M. Drop-tower experiments for capillary surfaces in an exotic container. *AIAA J., 30* pp. 134–137 (1992).

— Finn, R., and Vogel, T. I. On the volume infirmum for liquid bridges. Accepted by *Zeit. Anal. Anwend*, 1992.

— Fischer, B. S., and Finn, R. *Existence theorems and measurements of capillary contact angle.* Preprint, Dept. of Mathematics, Stanford University, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Convection and Morphological Stability During Directional Solidification*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-24-07-07

PRINCIPAL INVESTIGATOR: Dr. Sam R. Coriell
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TASK OBJECTIVE/DESCRIPTION

The general aim of this task is the study of the fluid flow, solute segregation, and interface morphology which occur during directional solidification. Control of solute segregation during solidification will allow preparation of materials with optimal properties. Modeling and numerical calculations will provide support for space flight experiments by J. J. Mavier, A. Rouzaud, and D. Camel of the Centre d'Études Nucléaires de Grenoble utilizing the directional solidification furnace developed by the MEPHISTO project. In collaboration with K. Leonartz of ACCESS B. V., calculations of convectives and morphological instability are being carried out for the succinonitrile-acetone system in support of space flight experiments on the IML-2 mission.

RESEARCH APPROACH

During the directional solidification of a binary alloy, solute inhomogeneities can arise from both fluid flow and morphological instability. In microgravity, buoyancy-driven fluid flow is reduced, and experiments to study the evolution of morphological patterns without the interference of fluid flow may be possible. We are carrying out theoretical studies of the interaction of fluid flow with the crystal-melt interface.

Included in the research are (a) calculations of cellular morphologies in the absence of fluid flow, (b) evaluation of the Seebeck voltage for cellular interfaces as a method for monitoring interface morphology in metallic alloys, (c) linear stability analyses of coupled interfacial and convective instabilities, and (d) calculations of the effect of time-dependent gravitational accelerations (g-jitter) on fluid flow during directional solidification. This proposed ground-based research will focus on providing theoretical interpretation and guidance for space experiments.

PROGRESS DURING FY1992

During directional solidification of a binary alloy at constant velocity, thermosolutal convection may occur due to the temperature and the solute gradients associated with the solidification process. For vertical growth in an ideal furnace (lacking horizontal gradients) a quiescent state is possible. The effect of a time-periodic vertical gravitational acceleration (or equivalently, of vibration) on the onset of thermosolutal convection has been calculated based on linear stability using Floquet theory.

Numerical calculations for the onset of instability have been carried out for a semiconductor alloy with Schmidt number of ten and Prandtl number of 0.1, with emphasis on large modulation frequencies in a microgravity environment, for which the background acceleration is very small. The numerical results demonstrate that there is a significant difference in stability depending on whether a heavier or lighter solute is rejected.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Brush, L. N., McFadden, G. B., and Coriell, S. R. Laser melting of thin silicon films, *J. Crystal Growth 114* 446–466, (1991).

— Coriell, S. R., Murray, B. T., McFadden, G. B., Wheeler, A. A., and Saunders, B. V. Convective and morphological instabilities during crystal growth: Effect of gravity modulation. *Proceedings of the Eighteenth International Symposium on Space Technology and Science* Kagoshima, 1992 p. 2155–2160.

— Hardy, S. C., McFadden, G. B., Coriell, S. R., Voorhees, P. W., and Sokorko, R. F. Measurement and analysis of grain boundary grooving by volume diffusion. *J. Crystal Growth 114* 467–480, (1991).

— Leonartz, K., Schmeling, H., Rex, S., and Coriell, S. R. Material science in the biological space-lab multi user facility NIZEMI. *In 4th Internationl Conference on Expermental Methods for Microgravity Materials Sciience Research.* R. A. Schiffman ed., Warrendale, PA, The Minerals, Metals & Materials Society, p. 161–167, 1992.

— McFadden, G. B., Murray, B. T., Coriell, S. R., Glicksman, M. E., and Selleck, M. E. Effect of modulated Taylor-Couette flows on crystal-melt interfaces: Theory and initial experiments. In *On the Evolution of Phase Boundaries, The IMA Volumes in Mathematics and its Applications, Vol, 43,* M. E. Gurtin and G. B. McFadden ed., New York, Springer-Vergla, p. 81–100., 1992.

— Saunders, B. V., Murray, B. T., McFadden, G. B., Coriell, S. R., and Wheeler, A. A. The effect of gravity modulation on thermosolutal convection in an infinite layer of fluid. *Phys. Fluids A4* , 1176–1189 (1992).

— Singh, N. B., Gottlieb, M., Henningsen, T., Hopkins, R. H., Mazelsky, R., Glicksman, M. E., Coriell, S. R., Duval, W. M. B., and Santoro, C. J. Effect of growth conditions on the quaility of lead bromide crystals. *J. Crystal Growth* 123 , 227–235 (1992).

— Singh, N. B., Gottlieb, M., Henningsen, T., Hopkins, R. H., Mazelsky, R., Glicksman, M. E., Coriell, S. R., Santoro, C. J., and Duval, W. M. B. Growth and characterization of lead bromide crystals. *J. Crystal Growth* 123, 221–226 (1992).

— Wheeler, A. A., McFadden, G. B., Murray, B. T., and Coriell, S. R. Convective stability in the Rayleigh-Bernard and directional solidification problems; High frequency gravity modulation. *Phys. Fluids* A3, 2847–2858 (1991).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Drop Microphysics*
RESPONSIBLE CENTER: LeRC PROJECT IDENTIFICATION: 674-24-05-35

PRINCIPAL INVESTIGATOR: Dr. Robert H. Davis
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TASK OBJECTIVE/DESCRIPTION

The overall objective of this research is to develop a comprehensive theoretical model of the relative motion, film drainage, and film rupture leading to coalescence of interacting drops dispersed in an immiscible fluid. Relative motion due to gravity, thermocapillary migration, and attractive van der Waals forces is considered.

Drop interactions and coalescence play key roles in a variety of phenomena, including liquid-liquid extraction, raindrop growth, multiphase flow, and processing of bimetallic melts within the liquid-phase miscibility gap. This research is concerned with the microphysics of coalescence and focuses on the near-contact interaction of a drop approaching a second drop or a surface or interface. The overall goal of this microphysical research is to predict deformation, film drainage, and collision rates using fundamental theoretical analyses. The research program is divided into three components directed at meeting this goal:

1. Near-contact relative motion for nearly spherical drops: The rate of approach and the onset of deformation and film drainage are examined for gravity-driven and thermocapillary-driven motion;

2. Evolution of drop deformation during film drainage: As the drops move closer, the natural evolution of the shape of the thin film separating them is predicted, as is the rate at which this film drains; and

3. Film rupture due to van der Waals forces: When the rate-limiting coalescence step of film drainage causes an unstable film to become very thin, then attractive van der Waals forces pull the drop interfaces together and cause rupture. The rupture time and the rupture mode are determined as functions of the system parameters.

Research Approach

A novel method which couples lubrication theory in the narrow separation gap and boundary integral theory for the drop phase is used. Matched asymptotic expansions are used for start times (small drop deformations) and long-times (draining film regions).

Progress During FY1992

It has been shown that a spherical drop will come into contact with another spherical drop (or a flat interface) in finite time under a constant driving force, such as gravity. This is in contrast to rigid spheres—they approach each other only asymptotically.

The evolution of the drop shape has been traced from an underformed state until a dimple is formed and long-time quasi-steady-state pattern is established. A dimple is always formed and for long-times, the film thickness is proportional to inverse powers of time. When Van der Waals forces dominate over gravity, the film ruptures at the nose of the drop prior to the formation of a dimple.

Graduate Students: 2 **Degrees Granted:** 1

Publications/Presentations

— Davis, R. H. Microhydrodynamics of particulate suspensions. *Adv. Colloid Interface Sci.* In press, 1992.

— Zhang, X., and Davis, R. H. The collision rate and small drops undergoing thermocapillary migration. *J. Colloid Interface Sci,,* 152, 548–561 (1992).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***Bubble-In-Liquid Mass Transport Phenomena in a Reduced-Gravity Environment***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-24

PRINCIPAL INVESTIGATOR: Dr. Kenneth J. De Witt
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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to determine the merits and feasibility of a space experiment to study bubble and droplet phenomena. The distinguishing characteristics of the research are that it involves mass transport phenomena of a gas bubble dissolving in a liquid, and also the transient and steady-state movement of a bubble or droplet due to thermocapillary, diffusocapillary, or combined temperature and concentration gradients. The behavior of multiple bubbles and droplets is also included in the experiment scope. The results will yield information that will advance the science of bubble and droplet dynamics and will have application to many problems in physical chemistry, materials science, and transport phenomena.

RESEARCH APPROACH

The approach consists of experiments and analytical and numerical modeling. Since mass transfer experiments cannot be done under normal gravity or short-term microgravity conditions, the present experiments have concentrated on observing surface-tension-driven flow in a bubble or droplet.

Ground-based and drop-tower experiments have included bubble and droplet motion due to an interfacial tension gradient resulting from a concentration gradient. The numerical modeling of the dissolution of a single bubble or of a moving bubble due to residual gravity effects was completed. Present modeling involves incorporation of thermal and concentration gradients at the interface. In addition, numerical modeling of the unsteady motion occurring both inside and outside of a translating bubble or droplet has been completed, and analytical work on transient gas-bubble motion has been initiated.

PROGRESS DURING FY1992

During the past year a short proposal for a Glovebox experiment was submitted. An enlarged proposal was prepared to respond to NRA-91-0SSA-17, "**NASA Research**

Announcement Microgravity Fluid Dynamics and Transport Phenomena: Research and Flight Opportunities," and submitted in November 1991. To aid in this effort, Dr. John Hegseth, a postdoctoral research associate, was hired in October 1991 to develop interferometric techniques to measure concentration gradients and diffusion coefficients. Further laboratory and drop-tower experiments on diffusocapillary phenomena were completed. The financial support for this experiment ended in May, 1992 and all work done after that date was under a no-cost extension to January, 1993. The current work being done on-site at LeRC by university faculty and graduate students will be terminated.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Del Signore, D. M., Oliver, D. L. R., De Witt, K. '., and Rashidnia, N., Experimental demonstration of diffusocapillary flow in an oil droplet. *J. Colloid & Interface Science 150*, no. 2, 584–588 (1992).

— Oliver, D. L. R. and De Witt, K. J. "Mass transfer from fluid spheres at moderate reynolds numbers: A boundary layer analysis." Presented at the 30th Aerospace Sciences Meeting, Reno, NV, AIAA Paper No. 92-0105, January 1992.

— Yung, C. N, De Witt, K. J., Brockwell, J. L., and Chai, A.-T. The transient motion of a sperical fluid droplet. *Cham. Engg. Comm. 110*, 163–186, (1991).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Studies of Two-Phase Flow Under Microgravity*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-18

PRINCIPAL INVESTIGATOR: Dr. A. E. Dukler
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TASK OBJECTIVE/DESCRIPTION

The objective of this study is to develop and experimentally verify theoretical models that predict two-phase flow regimes and characteristics in reduced gravity. The significance of the results will have application in space power, fluid and thermal management, and propulsion systems. Furthermore, by developing an understanding of the effect of gravity on flow regime characteristics and flow directions, it will be possible to have applications in the petroleum and nuclear industries.

RESEARCH APPROACH

The approach is to conduct reduced gravity experiments on the Learjet and in the 2.2-second drop tower and concurrently to develop models that predict the hydrodynamic characteristics of the gas-liquid flow as a function of the system operating conditions.

PROGRESS DURING FY1992

As a result of 39 flights, the flow-regime maps were significantly expanded, especially for the water-glycerine, and water-surfactant liquid solutions. These flights recorded data using the new conductivity probe electronics, new differential pressure transducers, and in a SAMS accelerometer. As a result of these tests, the transition criteria for the flow regimes are being revised. The Learjet rig was rewired to accommodate a new data acquisition and control system. Hardware has been procured and fabricated to facilitate using the rig for 1.0 in.- (2.54 cm.) inner-diameter test sections.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Dukler, A. E. "Two-phase flow at reduced gravity conditions: problems and possibilities." Presented at AIChE Winter Annual Meeting as keynote talk, November 20, 1992.

— Janicet, A., and Dukler, A. E. A model for gas-liquid slug flow at reduced gravity conditions. Accepted for publication by *AIChE Journal*, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Theoretical Influence of Microgravity on Critical Fluid Measurements*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-32

PRINCIPAL INVESTIGATOR: Prof. Richard A. Ferrell
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College Park, MD 20742-4111
PHONE: 9301) 454-3414

TASK OBJECTIVE/DESCRIPTION

This endeavor is tailored to theoretical support for current critical fluid microgravity space shuttle experiments Critical Fluid Light Scattering Experiment (CFLSE), and LeRC Critical Fluid Thermal Equilibration Experiment (CFTE), as well as for several other microgravity experiments in the definition phases. The results of the proposed study will both aid in the interpretation of and need the data from the microgravity experiments to confirm scientific conclusions. Those conclusions will greatly improve the cost effectiveness of the science from identified flight experiments.

RESEARCH APPROACH

The science activity will look at six areas; three each for classical fluids and for superfluid helium. For classical fluids they are: short and long time-scale equilibration driving forces, the anomalous dimension critical exponent of the density fluctuation correlation length, and shear viscosity near the liquid-vapor critical point. For superfluids, they are: a better prediction of the thermal conductivity temperature scaling, the frequency dependence of the shear viscosity, and provision theoretical insight into the unexpected temperature dependence of the second-sound velocity of ^{4}He near its Lambda transition.

PROGRESS DURING FY1992

A different description of the temperature dependence of turbidity near the liquid vapor critical point was formulated that allows clearer experimental access to a small exponent which manifests a correction to the customary Ornstein-Zernicke description. Improvement was made in the formulation of thermal conductivity of ^{4}He near its lambda-transition. Again, it is intended to aid experimental interpretation of low-gravity experiments.

A reinterpretation was made in the Boukari et al. published experiment, "Critical Speeding Up Observed." This work reflects the ongoing development of understanding of critical point equilibration dynamics. An unpublished investigation was carried out regarding the effects of g-jitter on correlation spectroscopy of the critical fluid in the Zeno space experiment.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ferrell, R. A. "Collective electron-electron interactions in metals." Seminar, University of California, Santa Barbara, April 1992.

— Ferrell, A. Correction to dynamic scaling for the lambda transition in liquid ^{4}He: III. Quasi-scaling at the natural boundary. In *From Phase Transitions to Chaos*. G. I. Kondor, L. Sasvari, and T. Tei, eds., Singapore: World Scientific, pp. 56–67, 1992.

— Ferrell, R. A. "Critical dynamics of fluids." Colloquium, Institute for Theoretical Physics, University of California, Santa Barbara, February 1992.

— Ferrell, R. A. Effect of fluctuating inertial forces on the critical dynamics of a pure fluid. *Annalen der Physik*. To be published, 1993.

— Ferrell, R. A. "Energy gap reduction by quantum phase fluctuations in thin superconducting films." Poster, Institute for Theoretical Physics, University of California, Santa Barbara, June 1992.

— Ferrell, R. A. *Limitations imposed by gravity on measurements of the critical viscosity of a pure fluid*. University of Maryland Physics Department preprint, 1992.

— Ferrell, R. A. "Quantum phase transition." International conference, Chairman and Organizer, Institute for Theoretical Physics, University of California, Santa Barbara, June 1992.

— Ferrell, R. A., and Hao, H. *Adiabatic temperature changes in a single-component fluid near the liquid-vapor critical point*. Preprint from sabbatical work at the Institute of Theoretical Physics, University of California at Santa Barbara, 1992.

— Ferrell, R. A. "Der Einfluss von Quantenfluktuationen auf die Suraleitfahigkeit in sehr Dunnen Schichten." Theoretical colloquium, University of Cologne, Germany, November 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Molecular Dynamics of Fluid-Solid Systems*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-29

PRINCIPAL INVESTIGATOR: Dr. Joel Koplik
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TASK OBJECTIVE/DESCRIPTION

The objective of this theoretical research is to examine the molecular behavior of fluids in small confinements and near boundaries, using molecular dynamics calculations and the statistical mechanics of classical fluids. It looks at time and spatial scales where continuum fluid mechanics provides no insight.

Examples investigated are static and flowing pure fluids near walls; freezing transition in small pores; the breaking and coalescence of droplet interfaces driven by gravity of flow; and droplet spreading on solid surfaces.

RESEARCH APPROACH

We will develop a transportable and robust molecular dynamics simulation code for vector and parallel processing mainframe computers. We will also develop a realistic molecular model of solid walls, that is, walls with correct thermal and mechanical behavior. This allows for true physics of wall interaction rather than idealized boundary conditions. We will explore and broaden the scientific relevance of molecular dynamics to fluid behavior of interest to microgravity science. A subgrant with J. Banavar at Penn State University will be utilized to execute some of the work.

PROGRESS DURING FY1992

The coalescence and rupture of interfaces have been studied by constructing microscopic versions of typical laboratory experiments on a computer. The spreading of atomic and diatomic liquids on a molecular solid was simulated in order to understand terraced spreading of liquids on solids.

A study of the dynamics of freezing in confined geometries has led to the elucidation of a novel mechanism of layer-by-layer freezing. The spinodal decomposition of initially well-mixed binary fluid mixtures has been studied both in the presence and absence of gravity. A study has begun to investigate contact angle hysterias in the motion of contact lines on chemically or structurally

disordered solids. Calculations of the nucleation of gas bubbles from impure mixtures have also begun.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Koplik, J. "Molecular dynamics of fluid-solid systems." Presented at the APS 1992 March meeting and at a Nordic Symposium in Denmark in May 1992.

— Koplik, J. "Phase transitions in porous media." Presented at the APS 1992 April meeting.

— Koplik, J., and Banavar, J. R. Molecular structure of the coalescence of liquid interfaces. *Science*, in press, 1992.

— Koplik, J., and Banavar, J. R. Molecular structure of interface rupture. Submitted to *Phys. Fluids A*, 1992.

— Ma, W.-J., Banavar, J. R., and Koplik, J. A molecular dynamics study of freezing in a confined geometry. *J. Chem. Phys.*, vol. 97, pp. 485–493 (1992) a.

— Ma, W.-J., Maritan, A., Banavar, J. R., and Koplik, J. Dynamics of phase separation in binary fluids. *Phys. Rev. A*, vol. 45, pp. R5347–5350 (1992).

— Maritan, A., Cieplak, M., Swift, M., Toigo, F., and Banavar, J. R. Random anisotropy Blume-Emery-Griffiths model. *Phys. Rev. Lett.*, vol. 69, pp. 221–224 (1992).

— Maritan, A., Swift, M., Cieplak, M., Chan, M., Cole, M., and Banavar, J. R. Ordering and phase transitions in random field systems. *Phys. Rev. Lett.*, vol. 67, pp. 1821–1824 (1991).

— Sokol, P. E., Ma, W.-J., Snow, W. M., Wang, Y., Herwig, K. W., Koplik, J., and Banavar, J. R. Freezing in restricted geometries. *Appl. Phys. Lett.*, vol. 61, p. 777 (1992).

— Yang, J.-X., Koplik, J., and Banavar, J. R. Molecular dynamics of drop spreading on a solid surface. *Phys. Rev. Lett.*, vol. 67, p. 3539 (1991).

— Yang, J.-X., Koplik, J., and Banavar, J. R. Terraced spreading of simple liquids on solid surfaces. *Phys. Rev. A*, in press, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Fluid Dynamics and Solidification of Metallic Melts (FDSMM)*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-33

PRINCIPAL INVESTIGATOR: Dr. Jean N. Koster
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TASK OBJECTIVE/DESCRIPTION

Fluid physics is the foundation of material solidification. The primary objective of the proposal is to develop a unique research capability for flow visualization of metallic and electronic melts. The research is focused on gallium melts.

The research will focus on the basic fluid physics phenomena of surface-tension-driven flows in materials processing. A multilayer melt system will be analyzed in order to access the possibility of reducing convective flow in one layer. Finally, the effect of the solidification on the fluid flow will be evaluated.

RESEARCH APPROACH

Progress toward achieving radiographic particle image velocimetry (RAPIV) of liquid metal convection has required extensive technological development. The RAPIV will be used to obtain system flow velocity vector fields using appropriate computational analysis. The goal of this effort is to design an elevated temperature RAPIV system capable of providing the first flow visualization of the liquid metal convection flow behavior. RAPIV has been used successfully to detect the solid-liquid interface of solidifying gallium and to observe tungsten particles in molten gallium.

Rectangular, two-dimensional test cell geometries for the series of high temperature RAPIV experiments have been chosen. Two aspect ratios (length:height) will be used: 4:1 and 1:1 (with unit integration depth). The 4:1 ratio is the classical "Hurle" geometry which is used often for comparative numerical studies.

The Integrated Convection Apparatus and Rotating Undercarriage Support (ICARUS) is a high-temperature (up to 1,000 °C) modular furnace capable of establishing any combination of vertical and horizontal temperature gradients in test cells of various geometries. This provides the capability to vector the gravity body force from 0° (horizontal) to 90° (vertical).

Progress During FY1992

Science requirements necessitate the need for accurate measurement and control of the test cell temperature gradient with both steady-state and time-dependent convective flow. A detailed investigation of the study and transient heat transfer characteristics of the test apparatus, including specific heating and cooling requirements, has been performed. The essential thermal control hardware has been designed and assembled, and a high-speed, 8-channel microprocessor-based process control system has been acquired and installed. The system is ready for use.

The development of neutrally buoyant, chemically inert tracer particles with high radiographic absorptivity is essential to the RAPIV project. A substantial ongoing portion of the development effort has been directed toward the design of the appropriate tracer particles; candidate particles are tungsten, coated with SIO_2 or glass coated with gold.

Graduate Students: 2 **Degrees Granted:** 1

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Nonlinear Drop Dynamics and Chaotic Phenomena*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-24-07-01

PRINCIPAL INVESTIGATOR: Dr. L. Gary Leal
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TASK OBJECTIVE/DESCRIPTION

The general objective of the UCSB portion of the research is to apply newly developed knowledge about the dynamical behavior of nonlinear systems, and newly developed methods for the numerical solution of large deformation free-boundary problems in fluid mechanics, to address a number of unexplained or unexplored issues associated with dynamics of levitated drops or bubbles in acoustic and electric fields. Specific objectives for the analysis of finite amplitude effects for bubble motion include:

1. Establishing conditions for existence of steady deformed shapes for both acoustic and electrostatic levitation. One point of special significance is the difference between the idealized zero-g environment where the drop shape will exhibit fore-aft symmetry along the axis of rotational symmetry, and the shape of a drop in a gravitational field where the fore-aft symmetry is lost.

2. Developing an understanding of modal coupling and instabilities associated with large amplitude deformations. In this part of the research, the interest is with time-dependent oscillations, both from an undeformed and a deformed equilibrium state, and subject to periodic forcing via either the acoustic or electric fields. Again, the effect of asymmetries in the shape associated with levitation in a gravitational field should be considered.

3. Developing an understanding of the conditions for transition between regular and chaotic oscillations, again associated with periodic forcing via either the acoustic or electric fields. The effects of mean deformation are again of special interest, including differences between zero-G and gravitational environment due to the mean asymmetries associated wit the latter case.

It should be noted that these general objectives incorporate most of the anomalous observations from previous studies of drop dynamics in the microgravity science program. As indicated in the original proposal, it is the existence of these

phenomena that largely motivated and suggested the importance of the present study.

The expected significance of this project is both as a very important contribution to the basic scientific understanding of drop dynamics under nonlinear, large-amplitude deformation conditions (where all previous theories are deficient and few systematic experimental studies have been done), and as a basis for an enhanced ability to manipulate and understand the limits of manipulating levitated materials in containerless process applications.

RESEARCH APPROACH

From the theoretical side, the proposed project has two basic elements: (a) Derivation and study of law dimensional model systems to obtain an initial framework for prediction of nonlinear dynamical phenomena and (b) numerical study of the full, large deformation fluid mechanics problem using boundary-integral techniques for studying the nondissipative limiting behavior, and boundary-fitted coordinate, finite-difference techniques for the general case. In both cases, similar studies have either recently been carried out (or are being carried out) for deformable (and compressible) gas bubbles in a liquid. Thus, the initial development of methodology for solution of the acoustically driven drop dynamics problem is a relatively straightforward adaptation of existing methods. The electrostatic levitation problem requires some additional modification to include the electric field calculation, but the corresponding governing equations, ets. have already been laid out be previous investigators. Once the problem formulation phase is completed, a detailed investigation of the three major objectives will be carried out, beginning with the problem of steady shapes in a steady levitation mode with and without gravity.

The theoretical work, by itself, can contribute in an important way to explaining previous "anomalous" observation in microgravity-oriented levitation experiments, and to providing a predictive framework that can be used to anticipate additional, as yet undetected phenomena that could be of great significance in material-levitation applications.

However, theory should not be viewed as capable of providing all of the answer. The low-order model systems study is expected to provide a global picture of possible nonlinear phenomena, but the models are often derived from small amplitude expansion theories, and thus, even if the low-order dynamical system is a faithful representation of the full problem in this limiting sense, it cannot be expected to capture all of the possibilities for large-amplitude deformations. Numerical solutions faithfully reproduce the complete physics, but provide only a case-by-case picture, and also suffer from limitations on resolution that make it difficult to capture any high-mode phenomena, or many fully three-dimensional effects.

Thus, experiments still must play a crucial role, and this project is an excellent example of a case where ground-based studies alone cannot be adequate. The ground-based work must always involve an asymmetric deformed base state of deformation, and for large amplitude deformation this will have very significant effects on both the steady state and time-dependent dynamics that cannot be completely assessed via theoretical studies. Thus, flight-based experiments must play a critical role in providing a basis for comparison with the ground-based experimental results. The latter can, of course, be much more comprehensive in scope. A limited set of studies for comparison purposes is an appropriate and realistic role for flight-base experiments. The flight-based experiments can also expand the range of parameters beyond that possible in the ground-based work.

PROGRESS DURING FY1992

One major area of progress during the past year, this representing funding for the ten-month month period from February 1992 to the present, has been to develop the modified codes necessary for the large-amplitude, numerical work. In particular, we have developed boundary-integral codes for the high-Reynolds-number limit (where we did not previously have a code), paying particular attention to minimizing numerical dispersion that otherwise leads to a dissipation of time-dependent deformation modes even in the potential flow limit where no dissipation should occur.

We have also worked on a mathematically correct method for the inclusion of weak viscous effects at the interface. The finite-difference code that was previously developed for gas bubble in a liquid, and for a liquid drop in a second liquid has been given a a relatively minor modification to treat the acoustically levitated drop problem, and a very significant effort is again being made to minimize numerical dissipation, which arises in this case primarily from the coupling between the fluid dynamics and the coordinate mapping required to maintain boundary-fitted coordinates for the time-dependent interface shapes. During this period, the postdoctoral student hired to work on this project, and the Ph.D. student, have also had to familiarize themselves with both the physical problems of interest, and the numerical methods that had been developed originally by students who are no longer in my group.

We have also initiated and completed some work associated with the nonlinear dynamics of modeling of the problem. First, in collaboration with Professor Kang (who did some of the original modeling of nonlinear dynamics effects in time-dependent bubble motions), we have completed a model study of the dynamics of a conducting drop in a time-dependent electric field. This work include prediction of the frequency modification due to mean deformation, the effects of resonant coupling between time-periodic oscillations of the electric field and the drop shape, and the conditions for transition to chaotic oscillations of the drop

shape. Second, we have completed studies of the nonlinear dynamics of compressible gas bubbles driven by a periodic acoustic stress on the bubble surface. This work is closely related to the analysis of drop dynamics in an acoustic field, and is also related to work at JPL on acoustic levitation of gas bubbles in a liquid.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Pool Boiling Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-37

PRINCIPAL INVESTIGATOR: Dr. Herman Merte
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TASK OBJECTIVE/DESCRIPTION

The program described here seeks to improve the understanding of the fundamental mechanisms that constitute nucleate pool boiling. The vehicle for accomplishing this is an investigation, including experiments to be conducted in microgravity and coupled with appropriate analyses, of the heat transfer and vapor bubble dynamics associated with nucleation, bubble growth or collapse, and subsequent motion.

Certain effects which can be neglected at normal Earth gravity, such as surface tension and vapor momenturn, can become quite significant in microgravity. Momentum imparted to the liquid by the vapor bubble during growth tends to draw the vapor bubble away from the surface, depending on the rate of growth, which in turn is governed by the temperature distribution in the liquid. Thermophoretic forces, arising from the variation of the liquid-vapor surface tension with temperature, on the other hand, tend to move the vapor bubble toward the region of higher temperature. The bubble motion will be governed by which of these two effects prevail.

The elements of nucleate boiling, for which research conducted under microgravity would advance the basic understanding, are summarized:

1. Nucleation or onset of boiling. Indications are that both heater-surface temperature and temperature distribution in the liquid are necessary to describe nucleation.

2. The dynamic growth of a vapor bubble in the vicinity of the heater surface. This includes the shape as well as motion of the liquid-vapor interface as growth is taking place. These are influenced by the liquid temperature distribution at the initiation of growth.

3. The subsequent behavior of the vapor bubble. This includes the motion, whether departure takes place or not, and the associated heat transfer.

RESEARCH APPROACH

In the proposed experiment, a pool of liquid, initially at a precisely defined pressure and temperature, will be subjected to a step-imposed heat flux from a semitransparent thin-film heater forming part of one wall of the container such that boiling is initiated and maintained for a defined period of time at a constant pressure level. Transient measurements of the heater surface and fluids temperatures near the surface will be made, noting especially the conditions at the boiling process in two simultaneous views, from beneath the heating surface and from the side. It is viewed that the conduct of the experiment and the data acquisition would be completely automated and self-contained. For the initial flight, a total of nine tests are proposed, with three levels of heat flux and three levels of subcooling. The outcome of the experiment is expected to include the following:

1. Observation of the liquid-vapor behavior, including bubble growth and motion as functions of heat flux, initial subcooling and time, and correlation with observed heater surface temperature variation;

2. Use of initial liquid temperature distribution at nucleation to compute vapor bubble growth rate for comparison with observation; and

3. Measurement of delay time to nucleation for correlation with nucleation theory.

PROGRESS DURING FY1992

The prototype hardware for the Pool Boiling Experiment was flown aboard the SL-J mission on September 12–20, 1992. Performance of the hardware was "near perfect." The data clearly reveal that pool boiling in reduced gravity (10^{-3}g) is a transient process and not a steady periodic one. At the higher-heat flux tests (8 w/cm^2), the temperature continued to increase as well as the vapor content. Tests conducted at the lower-heat flux levels resulted in a rapid speeding of the vapor across the heater as compared to the high-heat flux levels. In low gravity, the vapor bubbles adhered to the heater surface and were 1 cm to 5 cm in diameter. In normal gravity, the vapor bubbles lift off the heater surface due to buoyancy and are approximately 1.5 mm in diameter.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ervin, J. S., Merte, H. Jr., Keller, R. B., and Kirk, K. Transient pool boiling in microgravity. *International Journal of Heat and Mass Transfer*, vol. 35, No. 3, pp. 659–674, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Thermocapillary Convection*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-22

PRINCIPAL INVESTIGATOR: Dr. G. Paul Neitzel
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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to determine the stability and instability criteria for the basic state of thermocapillary convection in models of the float-zone crystal growth process. Energy-stability limits provide sufficient conditions for stability of a basic state, while linear-stability limits provide sufficient conditions for instability. The successful computation of such limits for an actual float-zone would identify conditions under which oscillatory convection (and undesirable striations in the final material) can be avoided.

RESEARCH APPROACH

The research associated with this project is being carried out in a variety of related, complementary areas: (a) extension of energy-stability results computed for thermocapillary convection in a half-zone assuming axisymmetric disturbances to include three-dimensional disturbances, (b) computation of linear-stability properties of the same basic state, (c) application of energy-stability theory of a half-zone basic state with a deformable free surface, (d) consideration of alternate (radiative) heat-transfer conditions at the free surface, and (e) direct numerical simulation of oscillatory thermocapillary convection in a half-zone.

PROGRESS DURING FY1992

The grant has closed out. During the last year, linear-stability calculations for the half-zone basic state with a nondeformable free surface have been completed. In light of recent results presented by European workers, who found stationary instability for Prandtl numbers near unity, some linear-theory calculations were repeated. No evidence of red eigenvalues, and thus stationary instability, have been found. A paper documenting the linear-theory calculations has been prepared. An energy-stability analysis has been performed incorporating the effects of radiative heat-transfer for the case of Rayleigh-Bernard convection between a pair of rigid parallel planes. The results indicate the expected finding that radiation is stabilizing to the motionless basic state.

Graduate Students: 7 **Degrees Granted:** 2

Publications/Presentations

— Hyer, J. R., Jankowski, D. F., and Neitzel, G. P. Thermocapillary convection in a model float-zone. *AIAA Journal of Thermophysics and Heat Transfer*, vol. 5, pp. 577–582 (1991).

— Mittelmann, H. D., Neitzel, G. P., Chang, K.-T., and Jankowski, D. F. Iterative solution of the eigenvalue problem in Hopf bifurcation for the Boussinesq equation. Proceedings of the Second Copper Mountain Conference on Iterative Methods, April 1992, submitted to *SIAM J. Sci. Stat. Computing*. 1992.

— Mittelmann, H. D., Law, C. C., Jankowski, D. F., and Neitzel, G. P. A large, sparse and indefinite generalized eigenvalue problem from fluid mechanics. *SIAM Journal of Scientific and Statistical Computing*, vol. 13, pp. 411–424 (1992).

— Neitzel, G. P., Chang, K.-T., Jankowski, D. F., and Mittelmann, H. D. Linear stability of thermocapillary convection in a model of the float-zone, crystal growth process. Presented at the Thirtieth AIAA Aerospace Sciences Meeting, Reno, NV, January 1992. Accepted by*The Physics of Fluids* , 1992.

— Neitzel, G. P., Chang, K,- T., Jankowski, D. F., and Mittelmann, H. D. "Linear stability of thermocapillary convection in a model half-zone." Presented at the Forty-Fourth Meeting of the Division of Fluid Dynamics of the American Physical Society, Scottsdale, AZ, November 1991.

— Neitzel, G. P., Law, C. C., Jankowski, D. F., and Mittelmann, H. D. Energy stability of thermocapillary convection in a model of the float-zone, crystal-growth process: Part 2, nonaxisymmetric disturbances. *The Physics of Fluids A.*, vol. 3, pp. 2841–2846 (1991).

— Neitzel, G. P., Mittelmann, H. D., Chang, K-T, and Jankowski, D. F. Linear stability of axisymmetric thermocapillary convection in crystal growth. In *Bifurcation and Symmetry*, (E. Allogwer, K. Bhmer, M. Golubitsky, eds.), *International Series of Numerical Mathematics*, vol. 104, pp. 275–284, Birkhuser, Basel (1992).

— Neitzel, G. P., Mittelmann, H. D., Law, C. C., and Jankowski, D. F. Stability of thermocapillary convection in float-zone crystal growth. In *Numerical Methods for Free Boundary Problems* (P. Neittaanmki, ed.), *International Series of Numerical Mathematics*, vol. 99, pp. 58–69, Birkhuser, Basel (1991).

— Neitzel, G. P., Jankowski, D. F., Mittelmann, H. D., Shen, Y., Law, C. C., and Chang, K-T. "Thermocapillary convection instability in microgravity crystal growth." Invited presentation at the VIIIth European Symposium on Materials and Fluid Sciences in Microgravity, Brussels, Belgium, April 1992.

— Neitzel, G. P., Chang, K-T, Jankowski D. F., and Mittelmann, H. D. "Linear stability theory of thermocapillary convection in a model of float-zone crystal growth." Presented at the Thirtieth AIAA Aerospace Sciences Meeting, Reno, Nevada, January 1992.

— Neitzel, G. P., Chang, K-T, Jankowski, D. F., and Mittelmann, H. D. "Linear stability of thermocapillary convection in a model half-zone." Presented at the Forty-Fourth Meeting of the Division of Fluid Dynamics of the American Physical Society, Scottsdale, Arizona, November 1991.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Industrial Processes*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-30

PRINCIPAL INVESTIGATOR: Dr. Simon Ostrach
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TASK OBJECTIVE/DESCRIPTION

The objectives of this study are to gain an understanding of the role of gravity in various industrial processes and to identify potential benefits of microgravity applications.

RESEARCH APPROACH

The approach is first to analyze various commercial processes and to evaluate gravity influences in the transport aspects of the processes, and second, to analyze the processes in a microgravity environment identifying potential commercial benefits. The commercial processes, or related commercial processes to be analyzed, include supercritical fluid extraction (SCF) processes, coating flows, formation of gas bubbles in liquid flow, dynamics of liquid-gas interfaces, transport phenomena in zeolite growth, and rotating electrochemical systems.

PROGRESS DURING FY1992

Accomplishments of this effort include:

1. A theoretical study of coating flows which showed that the film thickness in microgravity can be much smaller or much larger than in normal gravity. It was also shown that the coating is achieved much faster with greater precision and, consequently, a smaller coating device is needed in microgravity. A test setup for the study is being built.

2. Studies of the growth-in-gel mechanism during zeolite growth, both theoretical and experimental, showed that secondary nucleation occurs only in the gel portion. A correlation was derived which agrees with the observation that the gel shrinking to the bottom of the hydrothermal reactor is due to depletion of the flocculated gel particles. Also, a nondimensional parameter was derived as a criterion for secondary nucleation under normal gravity.

3. A theoretical model was developed for single-bubble formation in both terrestrial and microgravity environments. Two different flow systems were considered, a

co-flow system and a cross-flow system. Comparison of the theoretical predictions with available experimental results under normal gravity conditions was made and good agreement was demonstrated. In microgravity, two flow patterns, a bubbly and a slug flow, were classified.

4. A detailed scaling analysis was carried out for two representative electrochemical systems, a binary electrolyte and a well-supported electrolyte (Tenary system). Comparisons with reported numerical results were made and excellent agreement was demonstrated. A rotating apparatus has been built to study rotating electrochemical systems.

5. Numerical and analytical studies regarding g-jitter effects on the dynamics of liquid-gas interfaces in an open container in microgravity were carried out. The disturbing, damping, resonance, hysteresis, and depth effects on free-surface deformation were investigated at the resonant frequency. A g-jitter generates vigorous fluid motions and very large free-surface deformations. Hysteresis effects increase resonant frequencies but viscous effects alternate them.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 3

PUBLICATIONS/PRESENTATIONS

— Gluic, I. "Thermal convection in a rotating annulus." M. S. thesis, Case Western Reserve University, 1992.
— Jiang, H. D., Ostrach, S., and Kamotani, Y. "Scaling analysis of thermosolutally-driven natural convection in electrochemical systems." Presented at the Joint Conference at 3rd ISHT and 5th ISTP, Beijing, 1992.
— Kim, I.-H. "Modeling of bubble and drop formation in flowing liquids in terrestrial and microgravity environments." Ph.D. dissertation, Case Western Reserve University, 1992.
— Kim, I.-H., Kamotani, Y., and Ostrach, S. A modeling of bubble and drop formation in flowing liquids in microgravity. Submitted for publication in *AICHE Journal*, 1992.
— Zhang, H., "Gravity-dependent transport phenomena in zeolite crystal growth." Ph.D. dissertation, Case Western Reserve University, 1992.
— Zhang, H., Ostrach, S., Kamotani, Y. "Growth-in-gel zeolite crystallization and transport phenomena." Presented at the Tenth International Conference on Crystal Growth, August 1992.
— Zhang, H., Ostrach, S., and Kamotani, Y. "Transport phenomena in hydrothermal crystal growth of zeolites." Presented at the 1992 National Heat Transfer Conference, August 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Containerless Capillary Wave Turbulence*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-24-07-03

PRINCIPAL INVESTIGATOR: Dr. Seth J. Putterman
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TASK OBJECTIVE/DESCRIPTION

We are working toward the goal of studying turbulence in a broad-band spectrum of capillary waves that run around the surface of a containerlessly positioned drop of liquid. This experiment would constitute the first controlled measurement of turbulence in interacting waves. Consequences of this experiment range from the characterization of turbulence to the determination of universal properties of nonlinear systems and signal processing. The presence of a new propagating mode (second sound) in the capillary turbulence would have important ramifications with regard to attempts to achieve controlled thermonuclear fusion.

RESEARCH APPROACH

The problem consists of two components. They are (a) the generation of a turbulent distribution of surface ripples and (b) the detection and measurement of this state. These issues are being approached in ground-based experiments as well as in arrangements that simulate containerless fluids in microgravity. The ground-based experiments are being carried out in a fluid which is excited with a shake table. The preflight experiments are being developed with a levitated droplet of liquid.

PROGRESS DURING FY1992

We have succeeded in generating a broad band-frequency spectrum in capillary wave motion on the flat surface of fluid in a beaker. The waves are generated by vertical oscillation, and their frequency spectrum is detected with a thin wire probe. Since the diagnosis of turbulence also requires demonstration of the existence of a broad-band spectrum in wave number we have in addition developed a shadowgraph technique that can be used to yield a two-dimensional digitized image of the fluid surface. The Fourier transform of this image yields the degree to which the various wavelengths contribute to the motion.

A bispectrum analysis of the surface motion has also been developed. It show that the dominant contribution to the surface motion is indeed nonlinear. Between

these methods we will obtain a sensitive calibration of the surface dynamics. At present we are improving the means of detection by incorporating a high-resolution high-speed CCD and by increasing the contrast in the shadowgraph technique.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Wright, W., Hiller, R., and Putterman, S. Experiments on capillary wave turbulence. *J. Acoust. Soc. Am.* S2360, *92* , (1992).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Transport Processes Research*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-01

PRINCIPAL INVESTIGATOR: Dr. Jack Salzman
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TASK OBJECTIVE/DESCRIPTION

The objective of this task is to promote, foster, and enhance the quality and breadth of microgravity research conducted in the discipline of fluid physics.

RESEARCH APPROACH

The approach to achieving the task objective is to provide LeRC in-house support to (a) assist sponsored principal investigators in the conduct of their research (particularly when that research can benefit from unique expertise or facilities which reside at LeRC), (b) guide and assist in the definition of flight experiments, (c) assist in program planning and outreach programs in the external community, and (d) conduct in-house research to advance the understanding of transport and interfacial phenomena through exploitation of the microgravity environment.

PROGRESS DURING FY1992

1. In the area of thermocapillary bubble/drop migration, asymptotic results of the bubble velocity for large Marangoni numbers have been obtained using flow fields for both small and large Reynolds numbers. Interferometry was also used to show that the thermocapillary flow around stationary drops does not significantly alter the bulk liquid temperature field.

2. Success was achieved in demonstrating that the evaporation of a stationary droplet can induce thermocapillary flows as a result of Marangoni-Bernard instabilities. These flows were shown to dramatically affect the rate of the evaporation process.

3. Although problems were encountered in crucible sealing, tests demonstrated the ability of a real-time video X-ray system aboard the LeRC Learjet to visualize the dynamics of void formation during solidification of an aluminum sample in a low-gravity environment.

4. Numerical calculations have shown that the critical Marangoni number (Ma_c) for the onset of Marangoni-Bernard instability in a rectangular container increases as the container aspect ratio (AR) decreases. In a time-dimensional calculation, the most significant increase of Ma_c occurs at AR<1.2, where Ma_c increases almost exponentially with decreasing AR.

A reverse trend of Ma_c occurs between AR=1.3 and AR=1.45, where the Ma_c decreases as AR decreases. This anomaly is accompanied by a cell-pattern transition from a two-cell convection to a unicellular flow.

5. Reduced-gravity tests were initiated in the LeRC drop tower to examine the effects of a 3:4 expansion ratio in a conduit on two-phase flow regimes with a water-air system.

6. A drop-tower test rig was designed and assembled to study the interaction between fluid dynamics, heat transfer, and buoyancy in boiling of flowing thin liquid films. Test variables include the heating rate and the velocities of both the liquid in the film and the vapor adjoining the film.

7. Measurement capabilities developed in LeRC Fluid Physics Laboratory were used to support multiple flight projects. Accurate thermophysical property data such as the variation of surface tension (for both liquid-gas and liquid-liquid surfaces) and viscosity with temperature were produced for several flight-experiment fluids.

8. Extensive tests were conducted in the drop tower to examine both capillary flow in wedges and capillary flow driven by surface wettability. Results to date qualitatively agree with the limited existing predictions but also clearly show the need for both additional tests and extended theories.

9. A new multipurpose rig was brought on-line in a drop tower which enables studies of the effects of variable accelerations (i.e., variable in direction, frequency, and amplitude) on low-gravity fluid systems. Tests with this rig were successful in quantifying the destabilizing effect of off-axes excitation to a variety of circular "pinned" capillary surfaces.

10. J. C. Duh organized a professional short course on "Microgravity Fluid Dynamics," which was held at the sixth AIAA Annual Symposium on Microgravity Sciences and Space Processing in January 1992.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Arpaci, V. S., Selamet, E., and Chai, A. T. Thermocapillary instability of spherical shell. HTD-Vol. 180, *Fundamentals of Forced and Mixed Convection and Transport Phenomena* ASME, 1991.

— Chai, A. T., Rashidnia, N. and Arpaci, V. S. "Droplet evaporation with Marangoni instability induced convections." The 2nd Northern Ohio AIAA Mini-Symposium, May 27, 1992, Cleveland, OH.

— Chai, A. T., Rashidnia, N., and Arpaci, V. S. Marangoni instability induced convection in an evaporating liquid droplet. *Proceedings, VIIIth European Symposium on Materials and Fluid Sciences in Microgravity, Brussels, Belgium, April 12–16, 1992.*

— Chiaramonte, F. An initial study of void formation during solidification of aluminum in reduced gravity. *Journal of Spacecraft and Rockets,* October 1992.

— Dill, L. H., and Balasubramanian, R. Unsteady thermocapillary migration of isolated drops in viscous flow. *International Journal and Heat and Fluid Flow,* vol. 13, no. 1. pp. 78–85 (1992).

— Lee, J. and Thompson, R. Prediction of gas-liquid two-phase flow regime in microgravity. NASA Technical Memorandum, 1992.

— Rashidnia, N., Balasubramanian, R. and DelSignore, D. Interfacial tension measurement of immiscible liquids using a capillary tube. *AIChE Journal,* vol. 38, no. 4, pp. 615–618 (1992).

PATENTS — Weislogel, Mark, "Pulse Thermal Energy Transport/Storage System." July 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***Dielectric/Electrohydrodynamic Properties***
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-24-08-08

PRINCIPAL INVESTIGATOR: Dr. Dudley A. Saville
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TASK OBJECTIVE/DESCRIPTION

This investigation focuses on understanding those electrokinetic properties of particulate suspensions related to the so-called "electrohydrodynamic (EHD) effect," specifically, the dielectric constant and electrical conductivity. These properties are of crucial importance in defining the behavior of samples in various electrokinetic separation processes, specially those involving the purification of cell types.

RESEARCH APPROACH

Experimental and theoretical work will be carried out to understand the electrokinetic properties of particulate suspensions that produce the EHD effect. The dielectric spectroscopy technique developed at Princeton will be used to characterize model suspensions in support of work at MSFC, where a flight experiment is under development.

PROGRESS DURING FY1992

Most of our attention has focused on developing model particles which can be fully characterized using our dielectric spectroscopy technique.

We have found considerable electrophoretic mobilities with "electrically bare" particles. These are other uncharged particles which behave as though they have a large electrokinetic charge. This charge, found on both submicron-size particles and macroscopic surfaces, will make a substantial contribution to the electrokinetic properties of any suspension.

The first stage of our theoretical work on modeling the complex dielectric constant of dilute suspensions was completed and a paper accepted for publication in the *Journal of Chemical Physics.*

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Dunstan, D. E., Rosen, L. A., and Saville, D. A. Electrophoretic mobility of colloidal alkane particles in electrolyte solutions. *J. Chem. Soc. Faraday Transaction 88,* 2031–2033 (1992).

— Dunstan, D. E., Rosen, L. A., and Saville, D. A. Electrophoretic mobility of latex particles: particle concentration effects in low tonic strength solutions. *J. Colloid Interface Science 153* 581–584 (1992).

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***The Roles of Fluid Motion and other Transport Phenomena in the Morphology of Materials***
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-24-08-04

PRINCIPAL INVESTIGATOR: Dr. Dudley A. Saville
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TASK OBJECTIVE/DESCRIPTION

The objective is to find out how certain transport phenomena influence the morphology of crystalline materials. Two problems are under study: one deals with the effects of convection on the crystallization of pure materials, the other with the crystallization of proteins from solution. In the first study we are interested in how convection and other transport phenomena alter relations between the undercooling and the speed and stability of growth. In the second, we seek to find out why protein crystals grow as slowly as they do and how crystal morphology depends on the growth rate and crystal size.

RESEARCH APPROACH

A computation scheme has been developed which simulates the evolution of a needle-shaped crystal in an undercooled melt. It is being used to study the effects of interfacial resistances on microscopic solvability.

Experimental apparatus has been constructed to record the growth of protein crystals using a digital imaging system. Using model proteins, we studied the relations between crystal growth rate, size, and quality.

PROGRESS DURING FY1992

Theoretical work has disclosed a substantial effect of an interfacial transfer resistance on the operating point for a 2-D dendrite. We are now working to compare our theoretical results with experimental data in the literature.

The experimental work on lysozyme crystallization under quiescent and flow conditions is complete and the data analyzed. We have also completed theoretical work which takes account of electrostatic and dispersion forces between a protein molecule and crystal surface.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Saville, D. A., and Martin, C. A. "Kinetic effects in 2-d dendritic shape selection." AICHE Annual Meeting, Miami, November 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Capillary Containment of Liquids in a Microgravity Experiment*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-27

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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to explore the range of conditions for which fluid motion can enhance the stability of a free partially-free body of liquid against capillary instabilities, and to determine the motions generated when a geometrical configuration becomes unstable and results in rupture.

RESEARCH APPROACH

For the approach, linear stability analysis is used to predict stability conditions, and experiments attempt to confirm theory in a plateau apparatus. Auxiliary experiments and theory focus on aspects of stability and capture in thin-film systems.

PROGRESS DURING FY1992

This study has resulted in:

1. The discovery and mapping out, in a variety of contexts, of the windows in parameter space where hydrodynamics shear forces can stabilize capillary break-up in long cylindrical interfaces according to linear stability theory; rod flow (isothermal and thermocapillary-driven), tube flow, and core-annular rod flow. In particular, the physical mechanism of stabilization has been identified.

2. The designing, building, and testing of an apparatus capable of shear-stabilization in a parameter range where theory suggests stabilization may occur. Experiments show reasonable agreement with theory. In the course of the experimental investigation, a pressure-drop method of fine-tuning neutral buoyancy has been discovered.

3. The development of a simpler analog experimental system, the soap-film bridge, by means of which many of the fundamental influences of motion on stability may be studied. The soap film bridge has illustrated details of the collapse phenomenon never before documented.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Dijkstra, H. A. The coupling of interfacial instabilities and the stabilization of two-layer annular flows. *Phys, Fluids A 4*, (9), 1915–1928, 1992.

— Lowry, B. J., and Steen, P. H. Stabilization of an axisymmetric liquid bridge by viscous flow. In *Proceedings of the 42nd Annual Canadian Chemical Engineering Conference*, 1992.

— Steen, P. H. Capillary containment and collapse in low gravity: dynamics of fluid bridges and columns. In *Free Boundary Problems: Theory and Applications* . J. Chadam and H. Rasmussen, eds., vol. 3. New York: Longman-Pitman, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Mechanics of Granular Materials*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-24-07-06

PRINCIPAL INVESTIGATOR: Dr. Stein Sture
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TASK OBJECTIVE/DESCRIPTION

Ground-based displacement controlled triaxial experiments are conducted on a cohesionless granular material at the lowest effective confining pressures possible, that do not result in material instability, to assess constitutive properties, stability phenomena, and control parameters that will be applied to in-space experiments on 75 mm (diameter) and 150 mm (long) right cylindrical specimens. The ground-based tests on similar-size specimens are conducted in the range 3.5–69 kPa, while the microgravity tests will be conducted at effective confinement levels in the range 0.05–1.30 kPa. The purpose of these experiments is to gain a quantitative understanding of the mechanical behavior, including dilatancy, of cohesionless granular materials at different states of initial density, subjected to very low effective stress levels.

Efforts in support of design, development, test, and delivery of the flight apparatus that will be used in the Mechanics of Granular Materials experiments are presently underway. One flight and two reflight are currently planned.

RESEARCH APPROACH

The displacement-controlled mode of loading confined specimens was chosen mainly to maintain overall specimen-apparatus stability, while strain-softening resulting from continuous or discontinuous bifurcation and discontinuous deformation fields are allowed to take place. Optical and other noncontacting displacement-sensing techniques are used to measure specimen response during experimentation. Prescribed displacements are transmitted in terms of loading, unloading, and reloading historics, while volume change is measured in "drained" tests, and pore fluid pressure is measured in "undrained" isochoric tests. Confinement pressure is transmitted to the granular material assembly through a thin flexible latex membrane surrounding the specimen. A subangular and uniform Ottawa quartz sand constitutes the specimen.

Specimens tested both in space and on ground will be subjected to nondestructive and destructive (thin-slicing) testing to assess degrees of material uniformity and isotropy before and after experimentation. It appears that instability phenomena associated with specimens of certain configurations result in curved internal surfaces of localized deformation and high rates of dilatancy, whose structure depends on bifurcation mode.

PROGRESS DURING FY1992

The Science Requirements Document, which was completed in 1991, experiment design, management issues, and schedules were discussed in several meetings between HQ, Sandia National Laboratories (which is fabricating the MGM apparatus), and University of Colorado personnel, held during the year. The specimen and test configurations have been changed to accommodate physical requirements, and additional sets of experiments have been conducted to verify feasibility and to verify that the science is not compromised. Ground-based experiments are about to begin on the latest specimen configuration. Techniques for specimens preparation, handling, and dissection have been refined. Analysis and modeling procedures, especially in the area of evaluating material instability, have also been refined. Techniques for optically measuring displacements on the specimen's surface are also undergoing improvement.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Peric, D., Runesson, K., and Sture, S. Analysis of internal discontinuities in geomaterials. *Proceeding 9th Engineering Mechanics Conference, ASCE,* 1992, pp 292–296.

— Peric, D., Runesson, K., and Sture, S. Evaluation of plastic bifurcation for plane strain versus axisymmetry. *Journal of Engineering Mechanics, ASCE,* vol. 118, no. 3, pp. 512–521, (1992).

— Perkins, S. W., Sture, S., Ko. H.-Y., and Dialer, C. Modelherung von Tragwerken aus Regolith (Mondgostein) mittels Zentrifugonversuch. Journal Bautochnik, vol. 69, no. 11, pp. 644–650 (1992).

— Sture, S., Costes, N. C., and McTigue, D. F. Mechanics of granular materials at very low effective stress levels. *Proceeding 9th Engineering Mechanics Conference, ASCE,* pp 1035–1038, 1992.

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***Computational Studies of Drop Collision and Coalescence***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-24-05-07

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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to investigate the behavior of bubbles and drops in microgravity by full numerical solutions of the governing equations. Collision of drops and thermal migration of drops are studied in detail to provide essential input for material processing and fluid handling in space. These problems also serve as a test bed for refinements and extensions of the numerical technique that we are using, thus helping us develop the capability to predict accurately the behavior of free-surface fluid systems.

RESEARCH APPROACH

A numerical technique, based on explicit tracking of the interface between two immiscible fluids, is used in this study. The basic aspect of this method is described in the *Journal of Computational Physics*, vol. 100 (1992), p. 25. The unique aspect of the method is that it accounts fully for both inertia and viscous effects in both fluids and allows the inclusion of surface tension. It is also well suited for complicated interface geometries and has been implemented for fully three-dimensional flows. This method has now been extended to deal with the thermal migration, and the rupturing of thin films.

PROGRESS DURING FY1992

We have conducted extensive computations of the head-on collision of drops, establishing the dependency of the evolution on the governing parameters and, in particular, the sensitivity to the time of coalescence. The simulations show that it is important to predict this time accurately, and currently we are working on a "subgrid" model to predict this time in a physically correct way. We have also initiated work on non-head-on collisions of drops where the evolution is fully three-dimensional.

The thermal migration simulations are still two-dimensional. We have focused on the collective behavior of many drops and found rather remarkable pattern formation processes where the drops line up across the channel as they migrate toward the hot wall. This phenomenon, which has not been found before, has far-reaching implications for material processing.

Next year our focus will be mainly on the fully three-dimensional counterparts of these two problems.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: ***Theoretical Studies of Residual Accelerations in a Microgravity Environment; Stochastic Formulation of Fluid Flow Phenomena***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-36

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TASK OBJECTIVE/DESCRIPTION

This research involves a theoretical investigation of the effects that residual accelerations on board spacecraft can have on experiments conducted in a microgravity environment.

RESEARCH APPROACH

This effort will concern modeling the high-frequency, large-amplitude components of such residual accelerations (sometimes called g-jitter) as a stochastic of random process; that is, as a succession of random values of the intensity and orientation of the acceleration.

PROGRESS DURING FY1992

The general problem involving stability of a fluid surface separating two immiscible fluids subjected to residual accelerations of variable amplitude and orientation has been studied. Dr. Vinals has studied the prototypical case of a fluid surface separating two immiscible fluids of different density and viscosity.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 2

TYPE: Ground
DISCIPLINE: Fluid Physics
PROJECT TITLE: *Studies of the Dynamics of Charged Free Drops*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-24-07-09

PRINCIPAL INVESTIGATOR: Dr. Taylor G. Wang
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TASK OBJECTIVE/DESCRIPTION

The dynamic behavior of a charged liquid drop has been the subject of investigation. The basic assumption is that the charge essentially reduces the surface tension of a neutral drop; hence the shapes and stabilities of a liquid drop are greatly affected by the amount of charge presented on the drop surface. Various theories have been developed to predict the dynamic responses of a drop under different charge conditions.

However, two major obstacles make bias-free experiments rather difficult to achieve for ground-based experiments. One is the determination of charge quantity on a liquid sample. The proposed research objectives to be attained at Vanderbilt University in ground-based research are to optimize flight experiments and to advance our fundamental understanding of the dynamics of charged drops.

RESEARCH APPROACH

The study of the oscillation and rotational dynamics of charged liquid drops sustained by surface tension is interesting from both a fundamental standpoint and a practical standpoint vis-a-vis processing materials in space. The proposed ground-based experiments will help us to further the understanding of drop behavior and to optimize the approved flight experiments.

One of the major technical problems facing all charged-drop experiments is the determination of charge quantity on a liquid sample. To avoid the contamination and source loading problems, a noncontact charge-measuring technique is preferred. From basic physics, there is only one way to determine the potential of a charged object by noncontact means, and that is to measure the strength of the electrostatic field generated by the charge object. With precise calibration based on the geometry of the system and measuring distance, the field strength can be used to obtain the potential of the charged object.

PROGRESS DURING FY1992

Ground-based support studies on oscillating and rotating charged drops are underway at Vanderbilt University in an acoustic levitation chamber.

Study 1. The dynamics of drop oscillation. The present experiments are predominantly concentrating on studying the dynamics of charged free drops with negligible momentum interaction with the surroundings and drops with uniform surface charges. Acoustic forces will be solely used to levitate such drops. In addition, an immiscible levitation system will also be set up for making measurements on internal fluid flows in oscillating drops. Extensive flow visualiztion will be used for both qualitative and quantitative studies of drop dynamics.

Study 2. The dynamics of charged drop oscillation. A very-high-resolution charge-measurement system was developed at Vanderbilt University last year. This charge-measurement system has been incorporated into the ground-based acoustic levitator to study the dynamics of charged drop oscillations. A high-speed video system was used to determine the forced shape oscillation.

This year, variations of the drop oscillation amplitude decay changes in maximum oscillation amplitude viscosity and charge density will be examined. The freely decaying oscillations of charged drops on removal of acoustic excitation will be characterized. The effect of drop viscosity on drop behavior will be examined by using more viscous fluids like glycerine. Special attention will be devoted to the controlled study and characterization of the instabilities leading to mode coupling and to drop fission during large-amplitude oscillations.

Study 3. The dynamics of charged drop rotation. Rotation experiments will be performed on charged free drops. Earlier rotation experiments on drops in an acoustic levitation system have shown good agreement with theoretical predictions. However, the experiments on the rotating drops have shown only axisymmetric and 20lobed shapes. It is hoped that charged drops can be stably levitated over a reasonable length of time so that rotation experiments can be performed on them which will provide additional insights into this phenomena. Initially, a high viscosity fluid, like glycerin, will be used in the experiments. Drops will be rotated by acoustic torque.

Study 4. Conduction of combined oscillation and rotation experiments on charged drops. The objective of the ground-based studies will be to perform simultaneous oscillation and rotation experiments on charged free drops and to provide a scientific information base for future SpaceLab experiments.

Study 5. Development of internal flow field diagnostics technology. An immiscible drop levitation system was set up for the quantitative study of internal fluid motion in large drops (1 cm diameter). The proposed flow visualization technique will use the afterglow of UV excited phosphorescent tracer particles to retrieve vectorial information on particle motion. Zinc sulfide-coated, quasi-neutrally buoyant polystyrene particles (~50μ diameter) will be used as tracer. A UV strobe sheet or a pulsed nitrogen laser sheet (~1 mm thickness) will be used to illuminate and excite the tracer particles in the center plane of the drop. Both real-time video imaging and time-lapsed photography will be used to study internal motion.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Lin, K. C., and Wang, T. G. A method for noncontact drop charge measurement. AIAA paper no. 92-0018, January 1992.

PATENTS — Wang,, Taylor G. "Method and Apparatus for Non-Contact Charge Measurement." U.S. Serial No. 07/728.602.

TYPE: Ground
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Determination of the Correlation Length in Helium II in a Microgravity Environment*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-24-04-04

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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to measure finite size effects in the isobaric expansion coefficient near the lambda transition in liquid helium. Finite size effects are manifested as a rounding of the divergence in thermodynamic functions near a critical point as the correlation length increases toward the system size. We can thus test renormalization group theory predictions, universality assumptions, and boundary conditions.

We will measure the thermal expansion coefficient for liquid helium confined between parallel plates for a range of temperatures very near the lambda transition temperature (both above and below), a range of pressures from SVP to about 25 bar, and a range of plate separation distances.

RESEARCH APPROACH

We will measure the dielectric constant of helium confined between parallel plates as a function of temperature at constant pressure. Using the Clausius-Mossotti relation, the density and thus the expansion coefficient of liquid helium will be calculated. The experimental method involves two measurements (at a given temperature) of the balancing ratio of an audio-frequency ratio-transformer capacitance bridge, one with the sample capacitor empty and then one with it filled with liquid helium. Appropriate division of these ratios then yields directly the dielectric constant at that temperature.

The capacitor used to measure the dielectric constant is a parallel-plate design operated as a three-terminal device in a 1-kHz ratio-transformer bridge. The spacing between the electrodes is determined by a precision shim which can be easily changed. An identical capacitor is also mounted on the experimental platform and is operated empty as a reference capacitor. We expect to vary the thickness of the shims between 5 microns and 50 microns.

Initially germanium thermometry will be used for temperature control and measurement. This will allow us to easily cover a wide range of temperature and to gain familiarity with the experiment. At this stage we will want to reconcile our results with older, published data. High- resolution measurements will be made after installing a paramagnetic salt thermometer identical to that used by John Lipa in his lambda-point heat capacity experiment (LPE), which successfully flew on STS-52 in October of 1992.

PROGRESS DURING FY1992

The cryostat was first cooled down to liquid helium temperatures during FY 1992. After some modifications the refrigerator was made operational and could achieve a minimum temperature of 1.3 K. Further modifications to the input capillary filtering has made this device robust and problem-free. Modifications were made to the coaxial cables attached to the capacitors to allow more thorough heat-sinking. The run-time between liquid helium transfers was determined to be approximately 48 hours; however, it was demonstrated that helium could be resupplied during data taking with no measureable effects.

The dielectric constant in a 50 micron (bulk) gap capacitor was determined over the range 1.5 K to 4.2 K using a commercial capacitance bridge (General Radio model 1615A) and germanium thermometry. Subsequently the measurements were repeated using a custom ratio-transformer bridge and cryogenic reference capacitor. The absolute values of dielectric constant measured over this range of temperature by the two capacitance bridges differed by only 10 ppm and are consistent to within 60 ppm with earlier published data. Reproducibility between runs with the capacitors empty of helium was better than 2 ppm. Routines have been developed which fit cubic splines to the dielectric constant data, in appropriate form, to deduce expansion coefficient values.

A 500-micron spacer will be used next to obtain additional bulk helium data prior to inserting a 5-micron spacer to study finite size effects.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 4

TYPE: Ground
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Space Technology Experiments Platform (STEP)*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-24-07-10

PRINCIPAL INVESTIGATOR: Prof. C. W. Francis Everitt
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TASK OBJECTIVE/DESCRIPTION

The objective of the Space Technology Experiments Platform (STEP) experiment is to investigate the foundation of gravitational theory, the equivalence of inertial and gravitational mass. The STEP experiment may be thought of as a modern version of the experiment attributed to Galileo of dropping two weights from the leaning tower of Pisa. Any difference in the ratio of gravitational to inertial mass causes a corresponding difference in the rate of fall. The STEP experiment will be done in Earth orbit to a sensitivity of one part in 10^{17}, enhancing the measurement by a factor of one million over current measurement.

The experiment is one of four candidates for the next European Space Agency (ESA) medium-sized mission, to start around 1995. It is at the end a phase-A study being completed jointly by NASA and ESA. The mission, if selected, will be carried out jointly by the two agencies with an expected launch in the year 2000.

RESEARCH APPROACH

The satellite experiment compares the motions of twelve test masses in a drag-free satellite. Any difference in their motion at the frequency equal to the difference between orbital rate and the spin rate of the spacecraft indicates a violation of the Equivalence Principle. The masses' accelerations are measured with superconducting differential accelerometers based on SQUID technology, which can measure displacements as small as 10^{-13} cm. The experiment is cooled by 250 liters of superfluid helium that provides boiloff gas to operate a disturbance compensation of "drag-free" system for the spacecraft. The spacecraft will be placed in a 550-km Sun-synchronous orbit to minimize thermal effects.

Several co-experiments are planned, including a precise measurement of the gravitational constant, a test of the $1/R^2$ dependence of gravity, a spin-coupling experiment to look for the force due to the hypothetical particles called axions, a geodesy experiment to measure the shape of the Earth's gravity field, and an

aeronomy experiment to test questions related to atmospheric motion and density of orbital altitude.

PROGRESS DURING FY1992

The phase-A study is approaching its conclusion. Favorable solutions have been found for the major technical problems, including helium tide and momentum transfer and charging from particle radiation. A workable design for the superconducting accelerometers was available from the earlier assessment study, and has been simplified and extended in the present work. Significant changes were made in the concept of the co-experiments, especially the co-experiment to measure the gravitational constant, which now requires additional accelerometers, and provides an additional measurement of the $1/R^2$ dependence of gravity. A new co-experiment, the spin coupling or axion experiment, has been added, using an adaptation of the STEP accelerometer technology. Details of this work will be published by ESA in the forthcoming "Red Report."

We have continued to study in the laboratory questions related to the fabrication and performance of the apparatus, limited by time and manpower, which has been diverted largely to the paper phase-A study. These include fabrication and performance of the thin-film circuits needed for the magnetometers, flux motion issues, performance of the helium confinement system, and design and performance of a combined capacitance pickoff and electrostatic positioner.

GRADUATE STUDENTS: 4 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Mason, P. V., Israelsson, U. E., Petrac, D., Jackson, H. W., Worden, P., and Parmley, R. Technical challenges of satellite test of the equivalence principle mission. Space cryogenic workshop. 15–16 June, 1992, Accepted by*Cryogenics*., 1992.

TYPE: Ground
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Critical Transport Phenomena in Fluid Helium Under Low Gravity*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-24-02-01

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TASK OBJECTIVE/DESCRIPTION

Ground-based experiments will be carried out to study the temperature and density equilibration processes at constant average density ρ in a pure fluid (^3He) near its liquid-vapor critical point (T_c, ρ_c). Measurements are to be carried out for both the region above T_c (one phase) and below T_c (coexisting phases).

Such studies are very relevant to experiments on fluids under μg conditions, where investigations of static and dynamic properties near critical points are to be carried out. It is important to know how long a fluid system takes to come into thermodynamic equilibrium, and what are the basic mechanisms that control the equilibrium process. Later the measurements are to be extended to binary (^3He-^4He) mixtures.

RESEARCH APPROACH

Two types of cells are used. In the first one, the density stratification in the Earth's gravity field over a fluid layer height of 2 mm is measured via two thin horizontal superposed semitransparent capacitors that record the dielectric constant. The vertical density gradient is then derived via the Clausius-Mossotti relation. Stratification is recorded after a temperature change, and the resulting diffusion coefficient is determined as a function of temperature and average density. In a cell of the second type, the temperature equilibration in the middle of a fluid layer in the absence of convection will be measured after a rapid change in the cell temperature.

PROGRESS DURING FY1992

During spring 1992 the existing cryostat for work over a temperature range 1K–5K (previously used in the NASA-sponsored viscosity measurements) was modified to incorporate a temperature-regulated platform supporting the density equilibration cell. Electronic circuitry was installed for high-resolution stable temperature and dielectric constant measurements. Computer programs for temperature step control and automatic data acquisition and reduction were developed. The

apparatus was tested over a period of several months, and data-taking routines were developed and perfected. Initial density stratification data were obtained in the one-phase regime along the critical isochore and also in the two-phase regime.

Temperature steps of different sizes and sign were used and the stratification data were analyzed in a preliminary fashion. The stratification time was found to diverge as the critical point was approached from both the single-phase and the two-phase regimes. At a given temperature, it was found to be the same coming from either the colder or the warmer side. We expect to continue with data-taking along other isochores and along isotherms, and hope to present a scaling theme of our data.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Howald, C., Qin, X., Nham, H. S., and Meyer, H. Shear viscosity measurements of liquid ^{4}He and ^{3}He-^{4}He mixtures near the critical point.
J. Low Temp. Phys. 86, 1, (1992

— Qin, X., Howald, C., and Meyer, H. Shear viscosity measurements of ^{3}He-^{4}He mixtures above 0.5 K. *J, Low Temp. Phys., 87,* 731, (1992).

TYPE: Ground
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Critical Fluid Viscosity Measurement Experiment*
RESPONSIBLE CENTER: LeRC PROJECT IDENTIFICATION: 674-24-05-23

PRINCIPAL INVESTIGATOR: Dr. Michael R. Moldover
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TASK OBJECTIVE/DESCRIPTION

The purpose of this experiment is to develop a space experiment to produce archival data of Xenon closer to the liquid-vapor critical point than is possible in 1-g. The data will provide complementary results with the ZENO critical fluid light scattering experiment of Prof. R. W. Gammon at the University of Maryland to test the mode-coupling theory of critical phenomena and to provide guidance to hysterias group theory development on dynamic critical-point fluid behavior.

RESEARCH APPROACH

The task requires the use of a low-frequency, low-shear rate viscometer and a thermostat with approximately 27 μK temperature-control precision near room temperature. Viscosity measurements with an accuracy of 0.2% will be taken between μK and 600 mK of T_c. Sample loadings to within 0.3% of the critical density, and temperature gradients of less than 0.22 μK/cm, are also required to take advantage of the low-g environment. The sample geometry needs to be chosen and a heat transfer analysis must be done in order to establish thermal equilibration times that are realistic for shuttle flight timeline.

The experiment operation and data acquisition for the lab and flight hardware will be developed using full microprocessor automation. Critical point dynamics theorists will also be involved in the data analysis before and after flight.

PROGRESS DURING FY1992

A review in October 1991 authorized proceeding with flight experiment hardware conceptualization. A thermostat for temperature control has been designed and built. The viscometer cell was designed, built, and filled to the critical density. A comparison of electrostatic versus magnetic drives was made by direct tests. Detection of the viscometer's output signal was tested using both a lock-in and a spectrum analyzer. The science requirements were refined and a first draft of the Science Requirement Document was prepared for the Δ-Conceptual Design Review.

The issue of temperature and density equilibration was quantitatively addressed by model calculation. R. F. Berg and M. R. Moldover also shared in the IML-1 mission experiment "Critical Fluid Thermal Equilibration." This involvement greatly aided in defining temperature-time scenarios for CFVME. It brought attention to the boundary density distortion effects due to compressible fluid sample cooling.

GRADUATE STUDENTS: 0	**DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Berg, R. F. Wide-bandwidth viscometer for low-viscosity fluids. *Bull. Am. Phys Soc.*, vol. 37, no. 1, session M8 6, (1992).

— Berg, R. F., Wilkinson, A., Moldover, M. R., Eicher, L., Straub, J., and Gammon, R. "Density equilibration near the critical point of SF6 (TEQ/CPF on IML-1)." Poster at VIII European Symposium on Materials and Fluid Science in Microgravity, Bruxelles, Belgium, April 1992.

TYPE: Ground
DISCIPLINE: Fundamental Physics
PROJECT TITLE: *Studies in Electrohydrodynamics*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-24-05-25

PRINCIPAL INVESTIGATOR: Dr. Dudley A. Saville
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TASK OBJECTIVE/DESCRIPTION

The purpose of this work is to test and extend models of electrohydrodynamic processes involving fluid interfaces. Particular attention is given to the behavior of fluid globules and cylinders in systems with poorly ionized solutes at high (applied) field strengths. A microgravity environment may be necessary to test the theoretical models because experiments on Earth must be carried out with isopycnic systems to avoid sedimentation. The need to use isopycnic systems severely limits the range of fluid properties and phenomena that can be studied to test and extend theory.

The long-term objective of the research is the development of new ways to manipulate fluids, in particular, fluid interfaces. Externally applied electric fields offer a particularly attractive means of doing this because the electric stress is applied directly to the interfacial region.

RESEARCH APPROACH

The research has involved construction of mathematical models and experiments involving steady or oscillating fields with fluid globules and cylinders. The modeling work is intended to take specific account of charge transport processes. Experimental work involves use of digital imaging and analysis of steady and transient shapes of fluid bodies stressed by steady and transient electric fields.

PROGRESS DURING FY1992

The sample cell and high voltage electronics were used to study the behavior of a fluid cylinder stressed by an axial field. We had found that an axial field can either stabilize or destabilize the cylinder, depending on the properties of the two fluids. For example, using an electric field we were able to stabilize a cylinder whose length is more than 7 times as large as its radius; recall that the plateau limit is 3.14. An extensive study was carried out with both steady and oscillatory fields and a paper describing our work was accepted for publication in the *Physics of Fluids A*. We are currently analyzing our results in the context of G. I. Taylor's leaky dielectric model.

Our proposal to continue the work and prepare a science requirements document for a flight experiment was approved for funding.

GRADUATE STUDENTS: 1	**DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Vizika, O., and Saville, D. A. The electrohydrodynamic deformation of drops suspended in liquids in steady oscillatory electric fields. *J. Fluid Mechanics 239* 1–21, (1992).

— Sankaran, S., and Saville, A., "The stability of a fluid cylinder in an axial electric field." AICHE Annual Meeting, Miami, November 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: ***Glass Formation and Nucleation in Microgravity: Containerless-Processed, Inviscid Silicate/Oxide Melts, Ground-Based Studies***
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-26-07-01

PRINCIPAL INVESTIGATOR: Dr. Reid F. Cooper
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TASK OBJECTIVE/DESCRIPTION

There are two specific tasks involved in this research project:

1. Nucleation by internal oxidation or reduction of transition metal-bearing silicate melts. If a change in valence state of a transition metal cation within a silicate melt is associated with a change in its structural role within the melt, one might be able to effect internal homogeneous nucleation within the melt via a change in the external environment, for example, by a redox reaction. Critical to the hypothesis is the nature of transition metal cations to make the melt into a semiconductor: Conduction electrons or electron holes are majority defect species and thus serve to decouple cation and anion diffusion fluxes that occur in an oxygen chemical potential gradient. One consequence is that oxidation or reduction reactions can occur internally (i.e., within the body of the melt) instead of solely on the surface. These reactions can result in the destabilization of the melt such that crystallization reactions occur in finely (nm-scale) dispersed regions of the melt body (e.g., the formation of Fe^{3+} -bearing spinel precipitates via the internal oxidation of an originally Fe^{2+} -bearing aluminosilicate melt). One can thus create fine-grained glass-ceramics from what would normally be non-glass-forming melts. The environmental control required in the pursuit demands a containerless environment; the ability to ultimately produce controlled-shape parts from the uniform, fine-scale crystallization of a melt would take advantage of microgravity.

2. Internal nucleation of inviscid pseudobinary silicate melts via metastable liquid-phase immiscibility. Binary alkaline Earth oxide-silicate melts are highly exothermic. Nevertheless, the structural variations between highly polymerized (silica-rich) and poorly polymerized (silica-poor) silicate liquids result in the creation of composition zones (on the silica-rich end of the phase diagram) where a single silicate liquid is not stable. On the silica-poor end of the diagram, this immiscibility would be metastable.

As a consequence, if one can sufficiently undercool an inviscid, silica-poor melt, one could perhaps cause metastable amorphous-phase separation to occur prior to any crystallization. The phase separation could further promote the internal, fine (μm)-scale, uniform nucleation and crystallization of the material: The creation of unique glass-ceramic materials becomes a possibility. Containerless processing is crucial to secure the necessary amount of undercooling; a quiescent microgravity environment might further allow large bodies of inviscid melt to be so processed.

RESEARCH APPROACH

Two research approaches are employed for the two tasks:

1. Containerless processing for oxidation of $Fe^{2}+$ -bearing alkaline Earth aluminosilicate melts via aero-acoustic levitation (ALL). Small droplets (~3mm diameter) of ferrous iron-bearing calcium aluminosilicate glass, prepared initially by bulk melting in a controlled-oxygen activity furnace, are levitated and remelted using AAL and laser heating. The droplets thus formed are evaluated for their surface reactions, using Rutherford backscattering spectroscopy (RBS), and for their internal reactions using analytical transmission electron microscopy (AEM and TEM). The kinetics of the redox reaction are evaluated as functions of temperature, time, and oxygen activity, the latter controlled via the gas used as a levitation medium. The results of these experiments are compared to those done at low temperature on glasses of identical composition; with such a check, the study can be later extended to melts too inviscid to be glass formers. The nature of nucleation as affected by local oxygen fugacity will be explored using electron diffraction study of the internal oxidation front.

2. Drop-tube processing of pseudobinary silicate melts. Binary MgO-SiO_2 metasilicate compositions near the deep cristobalite (SiO_2)-enstatite ($MgSiO_3$) eutectic are melted in a drop tube. Initially fine, crystalline powder, the fine droplets are alowed by the degree of undercooling to experience metastable phase separation. Those droplets receiving sufficient undercooling to additionally penetrate the glass transition can be thermodynamically analyzed to explore the nature of nucleation in phase-separated amorphous materials. Primary analysis tools of the processing include secondary electron emission microscopy (scanning electron microscope), X-ray diffraction, TEM and electron microdiffraction, and differential thermal analysis and scanning calorimetry. These data should allow discrimination of the role of amorphous-amorphous interfaces on crystalline nucleation in the phase-separated amorphous droplets. The study will be extended to the binary Al_2O_3-SiO_2 system, the alumina-rich end producing highly inviscid melts that, if sufficiently undercooled, could produce interesting alumina/mullite glass-ceramics.

PROGRESS DURING FY1992

Progress on the two tasks is as follows:

1. Nucleation by internal oxidation or reduction of transition metal-bearing silicate melts. Oxidation experiments below the glass transition temperature were conducted on CaO-Na_2O-FeO-MgO-Al_2O_3-SiO_2 glasses that were initially prepared from a naturally occurring basaltic rock (Columbia River, Washington).

The kinetics of the oxidation process, analyzed by RBS, indicate that an internal oxidation process occurs in these glasses: Spectra indicate that oxidation causes Mg^2+, Fe^2+, Ca^2+, and NA+ to flux from the interior of the glass to the free surface, where they react with oxygen (and perhaps water vapor) in the environment; these fluxes must be charge-compensated by a counterflux of electron holes (Fe^2+ being thus transformed to Fe^3+ in the glass). While the physical process of oxidation is known with certainty via the spectroscopy, the structural changes in the glass accompanying the oxidation as well as the exact kinetic analysis requires TEM observations, which we are pursuing presently. Three suites of AAL experiments on Columbia River basalt were performed (in cooperation with Drs. Dennis Manthey and Richard Weber of Intersonics, Inc., Northbrook, Illinois); these experiments were notably successful for first attempts. Droplets created via laser melting of small rock specimens levitated on jet of rarefied argon (pO_2~10^{-6}) or dry air have been analyzed by RBS. The spectra thus produced suggests that oxidation reactions in the melt that are similar in form to those seen in the glasses do indeed occur, though oblation of alkali (and perhaps alkaline earth) ions in the processing environment make kinetic analysis difficult. Droplet specimens are also being prepared for TEM study at present. A suite of experiments on synthetic CaO-Na_2O-FeO-MgO-Al_2O_3-SiO_2 compositions are being prepared do as to avoid problems associated with loss of alkali ions.

2. Internal nucleation of inviscid pseudobinary silicate melts via metastable liquid-gas immiscibility. In work preceding the NASA Research Announcement (NRA), binary MgO-SiO_2 metasilicate compositions (approximately 50 mol.% MgO) were drop-tube processed in the 1,600 °C – 1,800 °C range. However, in work sponsored by this NRA, powders from these experiments that fused, metastable amorphous-phase-separated and crystallized were analyzed via X-ray diffraction (XRD) for phase composition in order to discern the relative percentages of the metastable orthosilicate (forsterite, Mg_2SiO_4) and stable metasilicate (enstatite, $MgSiO_3$) that formed. These data are presently being analyzed. Matriculation of a new graduate student on this project in September 1992 has seen recent recommencement of the drop-tube experiments on the binary magnesia-silica compositions. The next six months will emphasize thermochemical experiments geared to collecting statistical data on the relationship of amorphous phase separation to the kinetics of nucleation in droplets. We additionally anticipate initiation of experiments on Al_2O_3-SiO_2 compositions.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Cooper, R. F. "Oxidation, chemical diffusion and nucleation in iron-bearing silicate melts and glasses." Oral presentation at the Fourth International Symposium of Experimental Mineralogy, Petrology, and Geochemistry, Clermont-Ferrand, France, 16 April 1992.

— Fanselow, J. B. and Cooper, R.F. "Redox reactions, chemical diffusion and nucleation in natural basaltic glasses." Oral presentation at the V.M. Goldschmidt Conference, Reston, Virginia, 10 May 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Advanced Photonic Materials Produced by Containerless Processing*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-26-07-02

PRINCIPAL INVESTIGATOR: Dr. Delbert E. Day
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to: (a) use containerless melting to develop nonlinear optical glasses for use as ultrafast, all-optical switches and other photonic devices for communication and advanced computer application; and (b) investigate and compare the kinetics of nucleation and crystallization for these glasses—prepared by containerless melting—with the kinetics for the same glasses melted in a container.

The glasses that have been reported to possess the potential for nonlinear optical applications, such as the heavy metal oxide (HMO) glasses containing jPbO, Bi_2O_3 and Ga_2O_3, are made from highly fluid and chemically corrosive melts which readily crystallize during cooling. These typical characteristics not only decrease the glass-forming tendency for these melts, but develop unwanted color centers, primarily due to materials dissolved from the container. The conventional melting procedure for HMO compositions therefore results in colored and chemically in homogeneous glasses that are presently unusable for nonlinear optical applications. Containerless processing provides the opportunity to eliminate or suppress the heterogeneous nucleation and crystallization in a melt and increase the tendency for glass formation. Since no container is used, color centers caused by impurities dissolved from a container can be completely eliminated, even in a highly corrosive melt. The kinetics of nucleation and crystallization for HMO glasses prepared with and without a container will be investigated to determine, primarily, the temperature range for nucleation, the temperature for maximum nucleation, and the activation energy for crystallization. The nucleation and the crystallization data will be combined with the measured chemical durability to determine the stability of these glasses for practical applications.

At the completion of the ground-based work, the general plan is to conduct follow-on experiments with containerless melts in space, using compositions that appear most suitable to the operational parameters of whatever levitator furnace is

available. The purpose is to develop a glass with improved nonlinear optical properties by taking advantage of the reported observation that a glass prepared in a microgravity environment is chemically more homogeneous than an identical glass prepared on Earth. This observation from earlier space experiments can be verified by data from the present experiments, and the mechanism(s) of melt homogenization in the absence of gravity can be determined. The kinetic parameters for nucleation and crystallization determined for the space- and Earth-melted glasses are expected to yield a better scientific understanding for the relative role of heterogeneous and homogeneous nucleation in the processes of glass formation, nucleation, and crystal growth in fluid melts. Since an acoustic field is used to levitate and position melts for containerless processing, the proposed research will also attempt to identify any effect an acoustic field may have on the homogenization, nuclei formation, and crystal growth during a containerless glass-forming melt.

RESEARCH APPROACH

Initially, the investigation of nonlinear optical glasses started with HMO compositions in the system PbO, Bi_2O_3 and Ga_2O_3. The starting composition was chosen after discussions with Dr. William Dumbaugh at Corning, Inc., who has considerable experience with HMO glasses. Depending upon the initial results, other compositions containing TiO_2, Nb_2O_5, or TeO_2, which have the potential of yielding a high nonlinear refractive index and high infrared transmission cut-off (>8μm), will also be studied.

Glasses are prepared in containers of different materials, such as Pt, Au, and Al_2O_3, to determine which container has the highest corrosion resistance to these melts and will yield the best glass. Hot-pressed PbO, Bi_2O_3 and Ga_2O_3 samples of suitable composition will also be containerlessly melted and cooled at Intersonics, Inc., using their newly developed acousto-aerodynamic levitator/furnace. The critical cooling rate for glass formation, R_c (container) measured by the pendant-drop technique (spherical glass melt hanging from a thermocouple bead), will be compared with the R_c measured for containerless melt R_c (containerless) at Intersonics.

The ratio of R_c (container) to Rc (containerless) will be used to determine the improvement in glass formation for the containerless melt at 1-g. The kinetic parameters for nucleation and crystallization for these glasses (prepared with and without a container) will be measured by differential thermal analysis (DTA), and the crystallized phase(s) will be identified by XRD. The size and distribution of crystallized phase(s) will be determined by SEM and EDAX. Structural features of the glasses, such as cation coordination and oxygen bonding, which can be important to the kinetic parameters for crystallization will be investigated by NMR, XPS, and IR spectra.

Selected properties, such as the glass transition temperature, softening temperature, thermal expansion coefficient, density, refractive index, microhardness, chemical

durability, and the cut-off wavelength in the VIS and IR, also will be measured. The nonlinear refractive index will be measured only for the glasses that have the best combination of the above mentioned properties, and a nonlinear optical glass with optimized thermal, mechanical, nucleation, and crystallization properties will be developed at 1-g.

If flight opportunities become available, the optimum composition developed for nonlinear optical application from the ground-based investigation will be used in flight experiments. Hot-pressed spherical samples (6 mm to 8 mm in diameter) will be melted containerlessly in space and cooled at different rates. All of the properties measured for the 1-g glasses will also be measured for the post-flight samples. A comparison of these properties for Earth- and space-melted glasses will reveal the improvement in the optical and other related properties due to better chemical homogeneity for glass melted in space.

Any difference in the number, size, and distribution of nuclei in the Earth- and space-melted glasses can also be determined, the knowledge of which can be useful to understanding the mechanisms of glass formation and crystallization in melts processed in space and on Earth.

PROGRESS DURING FY1992

Following a series of discussions with Dr. Dumbaugh at Corning, Inc., a ^{40}PbO, $^{-35}Bi_2O_3$ and $^{-25}Ga_2O_3$ mol%, composition was initially chosen for the present investigation. When a well-mixed batch of this composition was melted in a Pt crucible at 900 °C for 30 min and quenched on a bronze plate, a glass with a dark brown color was obtained. This color makes the glass unsuitable for nonlinear optical applications. When analyzed by XPS, small Pt particles from the crucible were found throughout the glass, which indicates that HMO glasses are highly corrosive and contain a suspension of the metallic Pt particles. Changing the crucible from Pt to Au or alumina changed the color of the glass from dark brown to light brown (close to yellow), but the color could not be completely eliminated. During FY 1992, primary emphasis was on decolorizing this HMO glass to make it useful for nonlinear optical applications.

Several methods have been attempted to decolorize this glass. These include, in addition to using different container materials, melting the glass (850 °C to 1000 °C) for different amounts of time (30 min to 60 min) and in different atmospheres (air, oxygen, and nitrogen). Different decolorizing (CoO, Cr_2O_3, and CeO_2) and starting raw materials (nitrates and fluorides in place of oxides) also have been tried, but none of these attempts have proven entirely successful in decolorizing the HMO glasses. Attempts to find new ways are still continuing, and samples for containerless processing at Intersonics have also been made. It will be interesting to learn whether containerless processing can eliminate the color.

A few selected properties, density (d), thermal expansion coefficient (α), glass transition temperature (T_g), dilatometric softening temperature (T_f), and the cut-off

wavelength in the VIS (l vis) and IR (l ir), were measured as a function of composition for fifteen different PbO, Bi_2O_3 and Ga_2O_3 glasses. Except for the glass transition and softening temperatures, none of these properties changed significantly with composition. Replacing Bi_2O_3 by PbO decreased d, α, T_g and T_f, while α, l vis, and l ir remained unchanged. Replacing Bi_2O_3 by Ga_2O_3 decreased d, α, and 1 vis, but increased T_g and T_f. A similar change in the glass properties was also observed when PbO was replaced by Ga_2O_3. It appears that a substitution of Ga_2O_3 for either PbO or Bi_2O_3 has a larger effect on the properties of these glasses than when PbO is substituted for Bi_2O_3.

A part of this research program is to determine the nucleation and crystallization parameters for the HMO glasses. The parameters to be determined include the temperature range for nucleation, the temperature at which the nucleation rate is a maximum, the activation energy for crystallization, and the dimensionality of crystal growth. The techniques for these measurements have been developed at University of Missouri–Rolla, using lithium discilicate glass as a standard, and recently applied to determine the nucleation and crystallization parameters for a $Na_2O_2CaO_3SiO_2$. (NC_2S_3) glass.

The values for these parameters determined by the present technique for the NC_2S_3 glass are in excellent agreement with those determined by the older standard technique, which confirms the general applicability of the technique developed at the University of Missouri – Rolla. The advantages of the present technique over the older techniques are that it requires less time, only a small amount of sample is needed, and no special sample size or treatment (grinding and polishing) is needed. Measurements on nucleation and crystallization parameters for the HMO glasses are now in progress.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ray, C. S., and Day, D. E., "Nucleation and Crystallization in Glasses as Determined by DATA." Presented at the 4th Symposium on Nucleation and Crystallization in Glasses and Liquids, Evergreen Resort, GA 16–19 August, 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Kinetics of Phase Transformations in Glass Forming*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-26-08-07

PRINCIPAL INVESTIGATOR: Dr. Kenneth F. Kelton
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to develop computer models for realistic simulations of first-order phase transformations, in particular crystallization of liquids and glasses, and to design experiments to test those models. This research will lead to improved methods for the analysis of kinetic studies of these transformations, allowing, for example, kinetic parameters for nucleation and growth to be determined from peak profile studies of nonisothermal differential scanning calorimetry (DSC) measurements of crystallization. These new techniques will have wide applicability for phase transformation studies. In particular, they will allow real-time experiments of phase stability and transformation to be carried out in a microgravity environment.

Research Task Description: Glasses (primarily silicate based) that devitrify polymorphically by homogeneous nucleation are being studied experimentally and by computer modeling. Lithium disilicate ($Li_2O.2SiO_2$) is used for most calculations and experimental measurements, since the necessary kinetic and thermodynamic parameters are best known in that system. Other glasses studied include soda-lime silicate ($Na_2O.2CaO.3SiO_2$) and barium disilicate ($BaO.2SiO_2$). The computer modeling of glasses (primarily silicate-based ones) is done at Washington University. The silicate glasses are prepared by Drs. C. Ray and D. Day of the University of Missouri, Rolla, under a related contract; they also study the devitrification kinetics experimentally with differential thermal analysis (DTA). Transmission electron microscopy (TEM) and DSC measurements are made at Washington University under this contract.

PROGRESS DURING FY1992

The computer models describing nucleation and growth under isothermal and nonisothermal conditions by simulating directly the evolution of the nonequilibrium cluster distribution have been written and tested. The programs are now being used for a variety of investigations:

1. To assess whether a recent suggestion that the temperature of the maximum nucleation rate and its magnitude can be estimated from DSC studies of glasses that were preannealed at different temperatures;

2. To compare theoretical calculations and experimental measurements of DSC devitrification studies of glasses that were scanned through the nucleation zone (defined as a region of significant nucleation) at different scan rates; and

3. To assess the validity of analytical expressions commonly used to analyze nonisothermal kinetic data.

All points have been studied using lithium disilicate glass. The most surprising result is the remarkable agreement between the simulation results and the experimental data in investigations 1 and 2, dramatically verifying the validity of our approach. Armed with this agreement, we can make the first realistic critique of the existing techniques widely used to analyze nonisothermal kinetic data (investigation 3). This will be of interest to the entire materials community who use these techniques, often without a clear idea of the correct conditions for their use. We find that when used to analyze nucleation and growth data, all are fundamentally flawed, giving results that bear little resemblance to the kinetic parameters actually present in the transformation. We also find that the suggestion that the nucleation rate can be estimated from DSC transformation data depends on the glass studied. While this estimate is reasonably correct for lithium disilicate, it appears to be a strong function of the temperature dependence and magnitude of the growth velocity.

We are initiating additional studies to:

1. Model the other glasses mentioned previously (soda-lime-silicate ($Na_2O.2CaO.3SiO_2$) and barium disilicate ($BaO.2SiO_2$);

2. Probe the effects of particle size and nucleating agents;

3. Test the effects of preexisting nuclei resulting from different quench rates;

4. Investigate the possible effect of nonequilibrium viscosity on the devitrification behavior; and

5. Investigate the validity of an expression commonly used to simulate transient nucleation effects in isothermal transformations.

One paper has been written presenting a discussion, based on computer simulations, of the validity of the DSC method for estimating nucleation rates. These results were presented in an invited paper presented at the Fourth Symposium on Nucleation and Crystallization in Glasses and Liquids, held in Stone Mountain, Georgia, August 16–19, 1992. Several publications, including some written jointly with the Rolla group, are in preparation, or are planned in the immediate future.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Kelton, K. F. A computer model for nonisothermal transformations involving nucleation and growth. *Journal of Non-Crystalline Solids*. Manuscript in preparation, 1992.

— Kelton, K. F. Estimation of the nucleation rate by differential scanning calorimetry. *Journal of the American Ceramic Society, 75,* 2449–52 (1992).

— Kelton, K. F. An evaluation of the techniques for analyzing nonisothermal kinetic data obtained by DSC. *Journal of Non-Crystalline Solids.* Manuscript in preparation, 1992.

— Kelton, K. F. Transient nucleation in glasses. Invited paper, to appear in the *Proceedings of the Fourth Symposium on Nucleation and Crystallization in Glasses and Liquids,*. Accepted for publication, American Ceramic Society, 1992.

— Ray, C., Cull, T., Kelton, K. F., and Day, D. Nonisothermal devitrification studies (I): Lithium disilicate glass—Experimental and computer analysis. *Journal of the American Ceramic Society.* Manuscript in preparation, 1992.

— Ray, C., Cull, T., Kelton, K. F., and Day, D. Nonisothermal devitrification studies (II):$BaO.2SiO_2$—Experimental and computer analysis. To be submitted to the *Journal of the American Ceramic Society*, 1992.

— Ray, C., Cull, T., Kelton, K. F., and Day, D. Nonisothermal devitrification studies (II): $Na_2O.2CaO.3SiO_2$ — Experimental and computer analysis. To be submitted to the *Journal of the American Ceramic Society*, 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Chemical Vapor Deposition of High -To- Superconducting Films in a Microgravity Environment (I)*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-26-05-07

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TASK OBJECTIVE/DESCRIPTION

The basic goal of this research is to grow and process single-crystal high-temperature superconducting thin films under microgravity conditions. It is believed that microgravity will allow for unique growth conditions for vapor phase transport and for the formation of single crystalline materials during postprocessing to the superconducting phase.

RESEARCH APPROACH

Superconducting thin films will be grown by chemical vapor deposition in three different transport reactors in order to investigate the effects of gravitationally induced convection currents on the superconducting characteristics of the films. Different orientations with respect to gravity will be used.

PROGRESS DURING FY1992

A compact reactor for chemical vapor deposition of YBa2Cu307 superconducting films has been designed and is being assembled. The reactor has a single source wherein the precursor powders are stoichiometrically premixed and sublimed by a single quartz halogen lamp. Preliminary results show that a temperature of 420 °C may be achieved with the halogen lamp at the precursor powder within a Pyrex tube, which is in turn contained in an evacuated outer pyrex tube. Temperatures of 300 °C are necessary to evaporate the compacted precursor powders without decomposing them.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Kinetics of Phase Transformation in Glass Forming*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-26-08-08

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TASK OBJECTIVE/DESCRIPTION

The primary purpose of this research is to study and explain the critical issues for the nucleation and crystallization in glass forming systems. The reported data for the kinetic parameters that determine the overall nucleation and crystallization mechanisms are often difficult to interpret on the basis of existing theory. The interpretation becomes more difficult when a variation in the characteristics of the glass, such as the thermal history, composition, particle size of the sample, and concentration of the nucleating agent are taken into account. This is probably due to the fact that the theories that are presently used to analyze the isothermal and nonisothermal crystallization data for glass forming systems, are over simplified. Glasses are traditionally prepared by cooling a melt and are not in a state of stable equilibrium. Consequently, phenomena such as atomic mobility, cluster distribution, nucleation and crystal growth rate, and viscosity pertaining to the nonequilibrium state need to be accounted for to establish an accurate description of the phase transformations in glass forming systems.

The objectives of this research, therefore, are to (a) develop computer models for realistic simulations of nucleation and crystal growth in glasses, which would also have the flexibility to accommodate the different variables related to sample characteristics, and (b) design and perform nucleation and crystallization experiments to verify these models. This research will lead not only to improved methods for the analysis of kinetic parameters for nucleation and growth determined from the peak profile studies of nonisothermal differential scanning calorimetry (DSC) or differential thermal analysis (DTA) measurements of crystallization, but to determination of the relative merits and demerits of the theories presently used to study the phase transformations in glasses.

Glasses prepared in microgravity are reported to be more chemically homogeneous and more resistant to crystallization than identical glasses prepared on Earth, which indicates that the size and distribution of nuclei, and, hence, the mechanism of nucleation, are different in glasses processed in space and on Earth. This apparently

surprising observation from earlier space experiments can be verified from the results of the present investigation, once a realistic model for the nucleation and crystal growth in glasses is developed. The experimental and theoretical investigations of this research have been supported by NASA through separate contracts.

The experimental work is conducted at the University of Missouri-Rolla (NASA Contract NAG8-898, PI: C. S. Ray) and the theoretical work is conducted at the Washington University in St. Louis (NASA Contract NAG8-873, PI: K. F. Kelton).

RESEARCH APPROACH

Glasses (primarily silicate based) that devitrify polymorphically by homogeneous nucleation will be studied experimentally and by computer modeling. A lithium-disilicate ($Li_2O.2SiO_2$) glass will be used for most calculations and experimental measurements, since the necessary thermodynamic and kinetic parameters are available for this system. Other glasses that will also be investigated to verify the general applicability of the model include soda-lime-silica ($Na_2O.2CaO.3SiO_2$) and barium-disilicate ($BaO.2SiO_2$).

Crystallization experiments for the glasses will be conducted by DTA or DSC using the conditions used for computer modeling, such as the quench rate used to prepare the glass, sample weight, particle size of the sample, precrystallization heat treatment temperature and time, type and amount of nucleating agent, and DTA or DSC scanning rate. The experimental results will be compared with those predicted by the model. If flight opportunities become available, glasses of identical compositions will be prepared in space and the same crystallization experiments as were conducted for the Earth-melted control samples will also be performed for the returned flight samples.

The results from this research are anticipated to yield a realistic model for nucleation and crystal growth processes occurring in glass-forming melts, which would provide not only an improved scientific understanding for these processes, but allow a more accurate quantitative analysis of the thermal analysis data. This would help to explain several anomalous experimental results obtained for the kinetic parameters for crystallization and would lead to values that are more physically interpretable. The relative role of heterogeneous and homogeneous nucleation on glass formation can be determined and the reported observation that a glass prepared in low gravity is more homogeneous and more resistant to crystallization than an identical glass prepared at 1-g can be explained.

PROGRESS DURING FY1992

An experimental technique that uses nonisothermal DTA or DSC has been developed for determining the temperature range for nucleation and the temperature for maximum nucleation in a glass. The present technique, which requires in situ isothermal nucleation at different temperatures (for a fixed time)

prior to crystallization by DTA or DSC, requires fewer samples and is much faster than the technique commonly used for this purpose. The glasses investigated to date by this technique are $Li_2O.2SiO_2$ (LS_2), $Na_2O.2CaO.3SiO_2$ (NC_2S_3), and $BaO.2SiO_2$ (BS_2), and the results obtained for all these glasses are in close agreement with those reported in the literature. This technique provides not only the data for the temperature range for nucleation and the temperature for maximum nucleation of a glass, but predicts whether there is an overlap between the nucleation and growth rate curves for the glass (as a function of temperature).

A computer model describing nucleation and growth under isothermal and non-isothermal conditions has been developed at Washington University in St. Louis by directly simulating the evolution of nonequilibrium cluster distribution in a melt. This model justifies the experimental approach described above and, when applied to the LS_2 glass, yields the temperature range for nucleation and the temperature for maximum nucleation that are in excellent agreement with those determined by the present experimental technique. The model is now being tested for the NC_2S_3 and BS_2 glasses, the experimental data for which have already been obtained.

The effect of DTA/DSC scan rate on crystallization of the LS_2 glass was determined by scanning the glass through the nucleation zone (defined as a region of significant nucleation) at different rates followed by crystallization of the glass at a fixed heating rate. No change in temperature and profile of the crystallization peak was observed for this glass when the nucleation scan rate, α_n, was higher than 3 °C/min. For α_n <3 °C/min, the crystallization temperature decreased, and the height of the crystallization peak increased with decreasing α_n. This indicates that no new nuclei are formed in the LS_2 glass when the DTA/DSC scan rate exceeds 3 °C/min. This result is also in close agreement with that determined theoretically using the computer model developed in this research.

The following experimental and theoretical investigations are now in progress:

1. Check the validity of the nonisothermal thermoanalytical equations commonly used to determine the kinetic parameters for crystallization;

2. Determine the limit (above which no new nuclei are formed) of DTA/DSC scan rate for the NC_2S_3 and BS_2 glasses,;and

3. Investigate the effects of particle size, nucleating agents, preexisting nuclei (resulting from different quench rates), and non-equilibrium viscosity on crystallization of the LS_2, BS_2, and NC_2S_3 glasses.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ray, C. S., and Day, D. E., Nucleation and crystallization in glasses as determined by DTA. Presented at the 4th Symposium on Nucleation and Crystallization in Glasses and Liquids, Evergreen Resort, GA, August 16–19, 1992. *Proceedings of the 4th Symposium on Nucleation and Crystallization in Glasses and Liquids, American Ceramic Society.* In preparation.

— Ray, C. S., McIntyre, D. S., and Day, D. E. "Studies on nucleation and crystallization of glass by DTA." Paper #13-G-92, presented at the 94th Annual Meeting of the American Ceramic Society, Minneapolis, MN, April 12–16, 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Containerless Liquid Phase Processing of Ceramic Materials*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-26-07-03

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TASK OBJECTIVE/DESCRIPTION

This research uses the control of chemistry and nucleation achieved by containerless liquid-phase processing to study nonequilibrium phase formation and crystal growth. The work is intended to advance the basic understanding of the high-temperature chemistry of hard, refractory oxide and boride ceramics. Borides are of fundamental interest; they are a unique class of compounds which form highly covalent, complex crystalline structures.

Ground-based containerless experiments will enable non-equilibrium-phase-formation phenomena to be identified. This will allow candidate materials for more detailed investigation to be selected. Subsequent low-gravity containerless experiments will provide the high degree of control over molten specimens required for detailed studies and analyses of the liquids as well as crystal growth kinetics and solid-liquid phase relationships.

RESEARCH APPROACH

High-temperature liquid-phase processing will be achieved by aeroacoustic levitation in combination with laser-beam heating. The two groups of materials chosen for this work are: (a) rare-earth borides and (b) refractory oxides, for example, alumina. The major focus of the work will be on borides.

Metastable phase formation and epitaxial growth from molten rare-earth borides will be investigated. This unique group of materials is particularly hard and refractory; the atomic size differences between boron and rare-earth elements combined with the directional bonding between them result in compounds which exhibit a wide variety of crystal structures. Marginally unstable compounds are predicted to exist which will be accessed by nucleation of undercooled melts onto isostructural seed crystals. Amorphous phase formation will also be investigated by deep undercooling and possibly quenching of the higher melting borides.

Nonequilibrium phenomena displayed by undercooled oxide melts will also be investigated. It has already been found that the solidification behavior of undercooled liquid aluminum oxide differs greatly in oxygen and argon

atmospheres. Environmental effects on molten oxides will be investigated further by conducting containerless experiments in atmospheres of different oxygen potentials.

In addition to the materials research on borides and oxides, the investigators will undertake processing of materials provided by NASA-supported scientists at several other institutions during the first year of this project. These scientists are also interested in the processing and properties of oxide melts.

PROGRESS DURING FY1992

Work to date has been in four areas: (a) continuation of work on oxide materials started prior to the initiation of this contract, (b) equipment enhancements required for containerless experiments with boride materials, (c) synthesis and preliminary characterization of selected boride materials, and (d) aeroacoustic levitation processing of ceramic materials provided by other NASA-supported investigators.

(a) Work on oxide materials: Experiments with reluctant glass forming compositions in the calcia-gallia-silica system were conducted in collaboration with Professors Delbert Day and Chandra Ray from University of Missouri-Rolla. Detailed analyses of the results and further experiments were performed during the summer and a paper describing the glass formation, liquid optical properties, and fluid motion in the molten materials has been submitted for publication. This paper discusses the effects of quiescence on the undercooled melts, which is an important issue for microgravity science.

Work on the undercooling of liquid aluminum oxide was continued with experiments to evaluate the dependence of undercooling on the ambient oxygen pressure. Installation of a new data-acquisition system for the optical pyrometer has enabled precise measurement of the recalescence and arrest temperatures during solidification of the undercooled melt. Under a fixed oxygen potential, liquid aluminum oxide exhibited a highly reproducible nucleation temperature, approximately 300 °C below the melting point.

(b) Equipment enhancements: The aero-acoustic levitator has been equipped with a gas-flow system to continuously purge the region around levitated specimens with high-purity argon. Tests with copper and nickel specimens show that oxidation is significantly decreased but not completely eliminated with the purge operating. The system will be further improved by eliminating outgassing from virtual leaks in the gas purge.

Specimen temperature is monitored with an optical pyrometer operating at a wavelength of 650 nm. The pyrometer data-acquisition system has been modified so that data can be acquired at user-selected rates from 5 and 500 Hz.

A Centorr arc melter has been installed for synthesis of boride materials from mixtures of their component elements.

(c) Synthesis of borides: Refractory boride materials are hard and have high melting points. An arc melting method has been developed to synthesize specimens from high-purity powders. Arc melting on a water-cooled copper hearth produces sessile drops of molten material which solidify to produce specimens suitable for levitation.

Several specimens of lanthanum hexaboride have been prepared in the arc melter and levitated in the aeroacoustic levitator. The borides were laser-heated to temperatures above 2,000 K. Some oxidation occurred due to reaction with impurities in the inert gas used for levitation. Specimens of erbium, holmium and yttrium boride with various boron to rare-earth ratios have been prepared from powdered precursors. Chemical analyses will be performed on selected specimens to establish their final composition.

(d) Collaborative work: Three collaborations in the study of oxide melts are in progress.

Professors Delbert Day and Chandra Ray from the University of Missouri-Rolla have provided specimens of lead oxide-based glasses for melting and isothermal heating experiments. These experiments led to spalling, which was attributed to decomposition of residual carbonates when levitated specimens were heated. Additional specimens are being prepared and further experiments are planned.

Professor Reid Cooper and Mr. John Fanselow from the University of Wisconsin-Madison have used the aeroacoustic levitation facility to process basalt-based materials. Several natural and synthetic basalt specimens were successfully processed in air or argon atmospheres during two sets of experiments. A processing protocol is now established and further work is being planned.

Professor Bill Hofmeister and Mr. James Olive from Vanderbilt University have processed ceramic superconductor materials. Initial experiments achieved partial melting with rather large specimens. Additional work with smaller specimens is planned for mid-November.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— DeVos, J. K., Hampton, D. S., Merkley, D. R., Rey, C. A., and Weber, J. K. R. Containerless processing using various levitation techniques. *Jap. J. Space Res, 9,* 149–162 (1992).

— Nordine, P. C. "Containerless liquid phase processing and property measurements." Gordon Research Conference, High Temperature Chemistry, July 19–24, 1992.

— Weber, J. K. R. "Containerless experiments on liquid aluminum oxide." CNRS, Grenoble, April 17, 1992.

— Weber, J. K. R. Containerless processing of refractory ceramics. *Proceedings of the First Technical Interface Meeting for the Modular Containerless Processing Facility.* Jet Propulsion Laboratory Report JPL D-9370, 1992.

— Weber, J. K. "Undercooling and optical properties of aluminum oxide." CNRS, Grenoble, April 1, 1992.

— Weber, J. K. R., Anderson, C. D., Krishnan, S., Nordine, P. C., and Reed, R. A. Undercooling of liquid aluminum oxide. In preparation, 1992.

— Weber, J. K. R., Krishnan, S., Anderson, C. D., and Nordine, P. C. "Containerless liquid-phase processing of aluminum oxide by aero-acoustic levitation." Presented at TMS Annual Meeting, San Diego, March 2–5, 1992.

— Weber, J. K. R., Krishnan, S., Anderson, C. D., and Nordine, P. C. "Containerless processing and property measurements on liquid metals, alloys and dielectrics." Presented at VIII European Symposium on Materials and Fluid Sciences in Microgravity, Brussels, April 12–16, 1992.

— Weber, J. K. R., Krishnan, S., Anderson, C. D., and Nordine, P. C. "Containerless techniques for synthesis of non-equilibrium materials." Presented at TMS Annual Meeting, San Diego, March 2–5, 1992.

— Weber, J. K. R., Merkley, D. R., Anderson, C. D., Nordine, P.C., Ray, C. S., and Day, D. E. Enhanced glass formation for calcia-gallia (silica) compositions by containerless melt processing. *J. Am. Cer. Soc.*, submitted for publication, 1992.

— Weber, J. K. R., Krishnan, S., Anderson, C. D., Nordine, P. C., and Reed, R. A. Absorption coefficient of liquid aluminum oxide at 0.420 to 0.780 mm. In preparation, 1992.

TYPE: Ground
DISCIPLINE: Glasses and Ceramics
PROJECT TITLE: *Glass Forming Ability and Crystallization of Glass*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-26-04-02

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TASK OBJECTIVE/DESCRIPTION

The objectives are: (a) to identify compositions of glasses which could benefit from processing in microgravity and (b) to develop a theoretical framework to applicable to crystallization kinetics in 1-g and micro-g.

RESEARCH APPROACH

Both theoretical and experimental work are carried out in parallel; the latter includes glass preparations, in situ crystal growth measurements, and various surface and bulk diagnostics.

PROGRESS DURING FY1992

The relative importance of bulk and surface nucleation was studied as a function of cooling rate in the free-surface conditions relevant to containerless processing for both isothermal and non isothermal environments.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Bae, B., and Weinberg, M. C. Crystallization of Cooper metaphosphate glass. *J. Amer, Ceram. Soc.*, accepted 1992.

— Bond, D. A., Cheng, H.-Y., and Anderson, E. E. The growth of ZuS crystals by physical vapor transport; Indianapolis meeting of the APS, March 16–20, 1992. *Bull Amer. Phys. Soc.,37,* 666 (1992).

— Goktas, A. A., Neilson, G. F., and Weinberg, M. C. Crystallization of lithium borate glasses. *J. Mater. Sci. 27,* 24 (1992).

— Schneidman, V. A., and Weinberg, M. C. Induction time in transient nucleation theory. *J. Chem. Phys., 97,* 3629 (1992).

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- Weinberg, M. C. Transformation kinetics of particles with surface and bulk nucleation. *J. Non-Crystalline Solids 142,* 126 (1992).
- Weinberg, M. C. The use of site saturation and arrhenius assumptions in the interpretation of non-isothermal DTA/DSC crystallization experiments. *Thermochim. Acta 194,* 93 (1992).
- Weinberg, M. C., Zanotto, E. D., and Manrich, S. Classical Nucleation Theory with a size dependent interfacial tension: Li_2O-$2SiO_2$ crystal nucleation. *Phys. Chem. Glasses, 33,* 99 (1992).

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Microwave Materials Processing in Microgravity*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-25-04-07

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TASK OBJECTIVE/DESCRIPTION

The Microwave Materials Processing in Microgravity task objective is to apply the unique capabilities of microwave heating and positioning to process materials in microgravity. The task objectives will include (a) determination of the reaction mechanism, microstructure development, and physical properties associated with microwave synthesis of ceramics; (b) development and application of microwave techniques for monitoring the energy absorption during processing and measuring thermophysical properties of materials in microgravity, and (c) theoretical modeling of unique microwave heating and positioning capabilities in a microgravity environment.

RESEARCH APPROACH

There is a recognized need to produce advanced refractory ceramics that have higher melting temperatures and improved mechanical properties (such as strength and toughness). In recent years, ground-based experiments using microwave heating have demonstrated enhanced rates of sintering of ceramic materials, leading to new microstructures.

The synthesis of ceramics in a microgravity environment could provide the opportunity to produce contamination-free ceramics with controlled microstructures that lead to advanced structural applications. Microwave processing can heat many glass and ceramic compositions very rapidly to high temperatures, it can heat them more uniformly than other methods, and it is energy efficient.

Other important potential applications are crystal growth, and fiber pulling in space. Microwaves can generate a well-defined temperature gradient within a material, leading to the possibility of melting only the interior of a cylindrical sample, or leading to a radial gradient of the index of refraction upon solidification. By appropriate monitoring of the microwave parameters during processing one can also measure various sample properties as well as obtain energy absorption information which can be used to characterize the sample reaction and densification mechanisms.

We have recently demonstrated experimentally that microwaves can produce unique positioning forces. The ability to microwave heat and position a sample may lead to a new containerless technology that is ideally suited for controlled processing of materials in microgravity.

PROGRESS DURING FY1992

During this last year, we have (a) developed an advanced microwave absorption/thermal profile theory that calculates the steady-state microwave absorption and temperature profile within a sphere and applied this model to the processing of alumina demonstrated spheres, (b) demonstrated microwave sintering of 123 superconductors ($T \approx 1{,}050°C$), and (c) demonstrated experimentally the existence of the microwave force needed to containerlessly position a sphere at the center of a cylindrical cavity in a microgravity environment.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Barmatz, M., and Jackson, H.W. Steady state temperature profile in a sphere heated by microwaves. *MRS Microwave Processing of Materials III, 269*, 97, (1992).

— Barmatz, M., Watkins, J. L., and Jackson, H. W. Microwave processing of materials in microgravity. *30th Aerospace Sciences Meeting and Exhibit, AIAA Paper #92-0116*, January 1992.

— Jackson, H.W., and Barmatz, M. Method for calculating and observing microwave absorption by a sphere in a single mode rectangular cavity. *Ceramic Transactions 21*, 261, (1991).

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— Watkins, J. L., Jackson, H. W., and Barmatz, M. Measurement of microwave induced forces. *MRS Microwave Processing of Materials III, 269*, 151, (1992).

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Studies of Containerless Processing of Selected Nb-based Alloys*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-25-08-20

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TASK OBJECTIVE/DESCRIPTION

The research is presently focusing on determining the speed of solidification as a function of undercooling in the large undercooling regime.

RESEARCH APPROACH

Solidification velocity is measured on electromagnetically levitated specimens by monitoring the progression of the thermal field developed by recalescence. Velocity and temperature measurement are made with a custom-built device; it consists of a 1 X 38 lincox array of 4 mm by 0.96 mm photodiodes, two amplification stages, and data acquisition capability for both velocity and temperature measurements. The time when each detector senses the solidification front is recorded with a resolution of ten nanoseconds. The surface temperature of the levitated drop is measured by using the center photodiodes as a pyrometer.

PROGRESS DURING FY1992

The instrument for measuring velocity and melt temperature was built and applied to studies of pure nickel. Measurements were made over a range of undercooling from 8% of the equilibrium freezing point to 18%. At undercoolings less than 10% of the equilibrium temperature, the results agree in form with previous workers but markedly disagree at undercoolings greater than 10%. Previously reported results in the literature overestimate the solidification velocity of nickel at the large undercooling.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Bassler, B. T., Hofmeister, W. E., and Bayuzick, R. J. "Observation of materials beta solidification in the titanium aluminum systems." TMS Annual Meeting, San Diego, CA, March 1992.

— Bassler, B. T., Hofmeister, W. E., Bayuzick, R. J., Gorenflo, F., Bergman, T., and Stockem, L. Observation of alloy solidification using high speed video. *Rev. Sci. Instr., 63* (June 1992).

— Bertero, G. A., Hofmeister, W. E., Bayuzick, R. J., and Robinson, M. D. Containerless processing and rapid solidification of Nb-21 alloys of hypereutectic composition. *Metallurgical Transactions A, 22A* (November 1991).

— Bertero, G. A., Hofmeister, W. E., Bayuzick, R. J., and Robinson, M. D. Containerless processing and rapid solidification of Nb-21 alloys in the Nb-rich eutectic range. *Metallurgical Transactions A, 22A* (November 1991).

— Bayuzick, R. J. "Measurement of the solidification velocity in an undercooled free falling droplet." TMS Annual Meeting, San Diego, CA, March 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Dynamic Thermophysical Measurements in Microgravity*
RESPONSIBLE CENTER: HQ **PROJECT IDENTIFICATION:** 674-25-07-05

PRINCIPAL INVESTIGATOR: Dr. Ared Cezairliyan
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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to develop accurate millisecond-resolution dynamic techniques which, in a microgravity environment, will enable the performance of thermophysical measurements on high-melting-point electrically conducting materials in their liquid state at temperature above 1,500 K.

In addition to contributing to the advancement of general high-temperature science and technologies, the research is aimed at NASA flight support, specifically in the area of containerless processing. The research also has a strong component of shared technolgies with other NASA supported programs in the areas of specimen heating, energy measurements, temperature mapping, and various other sophisticated high-temperature measurement problems.

RESEARCH APPROACH

The research involves the development of a measurement system employing millisecond-resolution dynamic heating techniques for accurately determining, selected thermophysical properties (such as heat of fusion, specific heat, surface tension, and electrical resistivity) at high temperatures in a microgravity environment (KC-135 aircraft). The basic technique consists of resistively heating the specimen up to its melting point and above in about one second, by passing a large current pulse through it, while simultaneously measuring the experimental quantities with millisecond resolution.

As an integral part of the thermophysical measurements in microgravity, novel instruments are to be developed. These included high-speed multiwavelength and spatial scanning pyrometers. The multiwavelength pyrometer is capable of measuring radiance temperature at six wavelengths in the range 500–900 nm every 0.1 ms. The spatial scanning pyrometer is capable of measuring radiance temperature at about 1,000 points along a straight line (25 mm long) on the specimen with a complete cycle of measurements in about 1 ms. Both of these unique pyrometers are now operational.

PROGRESS DURING FY1992

Surface tension of tantalum at its melting temperature has been determined from the data obtained with the high-speed pulse heating system on board KC-135 aircraft.

The multiwavelength pyrometer has been used to measure (on the ground) the melting-point radiance temperature (at six wavelengths in the range 500–900 nm) of several tungsten specimens, yielding highly reproducible results to within ±1 degree kelvin.

A microsecond-resolution technique has been used to measure (on the ground) the heat of fusion of tungsten.

Testing of the spatial scanning pyrometer was completed and was used in preliminary experiments to measure temperature gradients in a rapidly heating tungsten specimen, providing data for diagnostic purposes and for determination of thermal conductivity, which will be a novel approach suitable for measurements at very high temperatures.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Cezairliyan, A., Foley, G. M., Morse, M. S., and Miiller, A. P. Six-wavelength millisecond-resolution pryrometer. In *Temperature*, vol, 6, J. F. Schooley, ed., (Am. Inst. Phys., New York, 1992), pp. 757–762..

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— McClure, J. L., and Cezairliyan, A. Measurement of the heat of fusion of tungsten by a microsecond-resolution transient technique. *Int. J. Thermophys.*, in press, 1992.

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— Miiller, A. P., and Cezairliyan, A. Radiance temperatures (in the wavelength range 519–906 nm) of tungsten at its melting point by a pulse-heating technique. *Int. J. Thermophys.*, in press, 1992.

— Miiller, A. P., and Cezairliyan, A. Surface tension of tantalum by a pulse heating technique. *Int. J. Thermophys.*, in press 1992.

— Miiller, A. P., and Cezairliyan, A. Radiance temperatures (in the wavelength range 521–906 nm) of molybdenum at its melting point by a pulse-heating technique. In *Temperature*, vol, 6, J. F. Schooley, ed., (Am. Inst. Phys., New York, 1992), pp. 769–774.

Type: Ground
Discipline: Metals and Alloys
Project Title: *The Dynamics of Disorder-Order Transitions in Hard Sphere Colloidal Dispersions*
Responsible Center: LeRC **Project Identification:** 674-25-05-18

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Task Objective/Description

The object of this research is to understand the fundamental nature of liquid-solid transitions. These fundamental studies are aimed at a microscopic understanding of the most basic static and dynamic aspects of liquids, solids, and the solidification process. The ideal system for such study is a set of hard spheres which, according to theory, should order as their density is increased past approximately 50%. The problem is that sedimentation prevents setting the density or attaining equilibrium of the sphere system. Research in microgravity may help overcome this problem.

Research Approach

The approach has focused on simulating low gravity by fluidizing a bed of specially prepared hard spheres (silica particles with short polymer coatings) with a counterflow of solvent.

Progress During FY1992

We have made great progress in studying a variety of different colloids suspended against gravity by the counterflow of the solvent; that is, with a fluidized bed. We have found the variation in sedimentation velocity resulting from hydrodynamic interactions and its effect or particle dispersion. We have observed crystallization of fluidized particles due to their Coulomb repulsion.

Graduate Students: 2 **Degrees Granted:** 0

Publications/Presentations

— Rutgers, M., Russel, W. B., and Chaikin, P. M. The elastic properties of colloidal sediments in a fluidized bed. *Bull. Am. Phys. Soc. 37,* 391 (1992).

— Xue, J-Z, Rutgers, M., Russel, W. B., Herbolzheimer, E., and Chaikin, P.M. Diffusion, dispersion, and settling of hard spheres. Submitted to *Phys. Rev. Lett.* 1992.

— Xue, J-Z, Rutgers, M., Russel, W. B., Herbolzheimer, E., and Chaikin, P.M. Hydrodynamic dispersions in hard-sphere fluidized bed. *Bull. Am. Phys. Soc. 37*, 706 (1992).

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Modeling Directional Solidification in Furnaces/Processes in the Microgravity Materials Science Laboratory*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-15

PRINCIPAL INVESTIGATOR: Dr. Arnon Chait
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TASK OBJECTIVE/DESCRIPTION

The objectives of this task are to develop a general-purpose numerical model for simulating directional solidification furnaces and to provide a consistent approach to process/sample parameter optimization.

RESEARCH APPROACH

The approach has been to develop required enhancements for simulating solidification processes with a finite element fluid, thermal and solutal solver; to develop numerical methodology for process optimization; and to develop new time-dependent, multidimensional, free-boundary algorithms.

PROGRESS DURING FY1992

Progress has included the addition of inverse design and optimization code which in turn uses our general purpose fluid or thermal analysis codes. A high-level inverse design and optimization code was added and specifically applied to the Programmable Multi-Zone Furnace (PMZF) configuration. The capability adds, for the first time, the explicit specification of the principal investigator science requirements (e.g., thermal gradients, interface shape, etc.) as an experimental design criterion.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— de Groh, H. C. III, and Kassemi, M. Effect of radiation on convection at moderate temperatures. Submitted to *AIAA J. of Thermophysics and Heat Transfer,* 1992.

— Yao, M., and de Groh, H. C. III. A 3-D FEM simulation of Bridgman crystal growth and comparison with experiments. *Numerical Heat Transfer, Part A: Applications.* September 1992.

— Yao, M., de Groh, H. C. III, and Chait, A. Application of the segregated solution approach in 3-D FEM modeling of crystal growth. *Advances in Finite Element Analysis in Fluid Dynamics II.* November 1992.

— Yeoh, G. H., de Vahl-Davis, G., Leonardi, E., de Groh, H. C. III, and Yao, M. A numerical and experimental study of natural convection and interface shape in crystal growth. Presented to the International Conference on Transport Phenomena in Processing, 1992.

— Young, G. W., and Chait, A. Surface tension driven heat, mass, and momentum transport in a float zone. Accepted for publication, *J. Crystal Growth,* 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Fluid Mechanics of Directional Solidification at Reduced Gravity*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-21

PRINCIPAL INVESTIGATOR: Prof. Chuan F. Chen
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TASK OBJECTIVE/DESCRIPTION

The primary objective of this research is to provide ground-based support for the flight experiment Casting and Solidification Technology (CAST), which was flown on IML-1 in January 1992. The secondary objective of the proposed research is to examine the stability phenomena associated with the onset of freckles and the mechanisms for their subsequent growth and decline (to eventual demise of some).

RESEARCH APPROACH

The focus is to study the convective motion and freckle formation during directional solidification of NH_4CL from aqueous solution at simulated parameter ranges equivalent to reduced gravity. This will involve state-of-the-art imaging techniques and mathematical models for the prediction of the observed phenomena.

PROGRESS DURING FY1992

Comprehensive experimental results on the directional solidification of NH_4C1 solution have been obtained. Using flow visualization techniques and time-lapse motion pictures, convection motion in the mushy zone before and after the onset of plume convection has been observed. The effect of gravity modulation on the onset of instabilities in a double-diffusive layer with gross-diffusion has been analyzed using linear stability analysis with Floquet theory.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Chen, C. F. Convection in the mushy zone during directional solidification. In *I nteract ive Dynamics of Convection and Solidification,* Davis, Huppert, Muller, and Worster, eds., pp. 139–141. The Netherlands: Kluwer Academic Publications, 1992.

— Chen, C. F. Surface tension effects on the onset of double-diffusive convection. In *Microgravity Fluid Mechanics,* H. J. Rath, ed., pp. 325–333. New York: Skpringer-Verlag, 1992.

— Chen, C. F. Viscosity effects on the directional solidification of NH_4Cl solution in a Hele-Shaw cell. *Physics of Fluids A.*, vol. 4, no. 9 (Gallery of Fluid Motion), 1992.

— Chen, C. F., and Chen, F. Onset of salt-finger convection in a gravity-gradient. *Physics of Fluids A.*, vol, 4, no. 9, (Gallery of Fluid Motion), 1992.

— Chen, C. F., and Su, T. F., Effect of surface tension on the onset of convection in a double-diffusive layer. *Physics of Fluids A.*, vol. 4, pp. 2360–2367, 1992.

— Chen, C. F., and Ehrhard, P. "Onset of chumney convection in a mushy layer generated in a Hele-Shaw cell." Presented at the 45th annual meeting of APS-DFD, Tallahassee, FL, November 1992.

— Landis, M. A., and Chen, C. F."Solid fraction distribution in a mushy layer by computed tomography." Poster presentation in the Gallery of Fluid Motion, 45th annual meeting of APS-DFD, Tallahassee, FL, November 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Modeling of Coalescence*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-35

PRINCIPAL INVESTIGATOR: Prof. Robert H. Davis
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TASK OBJECTIVE/DESCRIPTION

The overall objective of this research is to develop models to predict drop-size-distribution evolutions due to droplet collisions and coalescence during processing within the miscibility gap of bimetallic liquid-phase-miscibility-gap materials. When bimetallic liquid-phase-miscibility-gap materials are cooled through the miscibility gap, droplets rich in one of the metals form in the liquid matrix rich in the other metal. Droplet coalescence and phase segregation then occur due to buoyancy, thermocapillary, and other nongravitational mechanisms. Drop-size distribution evolutions in time are calculated by population dynamics models.

RESEARCH APPROACH

In the population dynamics models, continuous drop-size distributions are discretized into a large number of categories. The formation and destruction of drops in each size category is tracked. Drop motion due to gravity sedimentation, Marangoni migration, Brownian motion, and bulk flow are considered individually or collectively.

Classic expressions attributed to Smoluchowski for the collision rate between drops (that are required in the collision kernels opposing in the population dynamics models) are improved to include attractive, repulsive, and hydrodynamic interactions between drops. In particular, trajectory calculations are used to predict collision efficiencies.

PROGRESS DURING FY1992

A computer program has been completed for solving the population dynamics model to follow droplet size evolutions with time in homogeneous dispersions due to collisions arising from gravity sedimentation, Marangoni migration, and/or Brownian motion. Some of the key results are that a bimodal initial distribution will exhibit much more rapid coalescence due to gravity sedimentation or

Marangoni migration than will a unimodal initial distribution. A unimodal initial distribution will evolve into a bionodal distribution, then into a shifted and broadened unimodal distribution, and the coalescence may be greatly reduced by antiparallel alignment of the gravity vector and the temperature gradient.

Collision efficiencies for Brownian motion and gravity sedimentation for drops having a range of viscosity and radius ratios have been computed both in the presence and absence of attractive forces. A key result is that, in contrast to rigid particles, spherical liquid drops have nonzero collision efficiencies in the absence of attractive forces.

Theoretical work on combined mechanisms for drop coalescence has been focused on buoyancy and Marangoni motion with the gravity vector aligned antiparallel to the temperature gradient. The collision efficiencies for thermocapillary motion are larger than those for gravity motion, because of the more rapid decay of the velocity fields created by drops undergoing thermocapillary motion, provided that the thermal conductivity of the drops is not too large.

Our results show that there is a finite region in parameter space for which no collisions occur. This is because the interaction of two drops due to thermocapillary migration decays more rapidly with the separation distance R (as $1/R^3$) than does the interaction of two drops in gravity motion (which decays as $1/R$). As a result, the large drop which moves toward a small drop below it due to gravity may reach a separation distance where the initially weaker thermocapillary effects just balance the buoyancy-driven relative motion, and so the separation distance then no longer decreases.

Time scales have been determined to phase segregation and drop coalescence, together with criteria for predicting whether or not significant coalescence will occur prior to phase segregation. A computer model is being developed to solve population balances for drop size distributions which show that the phase segregation rate initially increases due to coalescence and subsequently decreases as the large drops migrate out of suspension.

Physical data on a variety of bimetallic and transparent immiscibles have been collected, and dimensionless parameters presenting various effects have been tabulated as functions of drop size. Data on composite Hamaker constant (for van der Waals attraction) and temperature coeffiicients of interfacial tension (for thermocapillary migration) are sparse, and order-of-magnitude estimates are typically used. Calculations of collision efficiencies have been made for bismuth drops in a zinc melt and for ethyl salicytate drops in diethylene glycol.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Davis, R. H. Microhydrodynamics of particulate suspensions. *Adv. Colloid Interface Sci.* In press, 1992.

— Zhang X., and Davis, R. H. The collision rate and small drops undergoing thermocapillary migration. *J. Colloid Interface Sci,* vol. 152, pp. 548–561 (1992).

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Theory of Solidification*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-16

PRINCIPAL INVESTIGATOR: Prof. Stephen H. Davis
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TASK OBJECTIVE/DESCRIPTION

The objective of this work is to obtain a quantitative understanding of the effects of various factors present during solidification on the solid/melt morphology.

RESEARCH APPROACH

In the approach, nonlinear stability theory, asymptotic, and numerical methods are all used to investigate the stability of the coupled systems describing the directional solidification of binary systems from the melt.

PROGRESS DURING FY1992

Progress during the past year has been made in many areas of solidification, including hydrodynamics and the behavior of cells and dendrites. The effect of morphology of Soret convection was examined experimentally and theoretically. The traveling waves normally associated with Soret convection are generally eradicated by the presence of a solid-liquid interface that can melt and freeze. A survey article has been written on the interaction of flow and morphology. It will appear in the *Handbook of Crystal Growth*.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Anderson, D. M., Worster, M. G., and Davis, S. H. "The solidification of a liquid droplet on a cold plate." 44th Annual Meetingf of the Division of Fluid Dynamics, American Physical Society, Tempe, AZ., 1992.

— Braun, R. J., Merchant, G. J., Brattkus, K., and Davis, S. H. "Nonlinear oscillation in rapid directional solidification." 44th Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Tempe, AZ, 1992.

— Braun, R. J., Merchant, G. J., Brattkus, K., and Davis, S. H. "Nonlinear analysis rapid solidification." Tenth International Conference on Crystal Growth, San Diego, CA, 1992.

— Davis, S. H. "Rapid solidification of a binary alloy." Department of Mathematical Sciences, University of Akron, 1992.

— Davis, S. H. "Microscale coupling of solidification and flow." In Interactive Dynamics of Convection and Solidification, NATO Advanced Research Workshop, Chamonix (Plenary lecture), 1992.

— Davis, S. H. "Strongly nonlinear oscillations in rapid directional solidification." Department of Mathematics, University of Utah, 1992.

— Davis, S. H. "Instabilities in rapid solidification." Department of Metallurgical and Materials Engineering, Illinois Institute of Technology, 1992.

— Huntley, D. A., and Davis, S. H. "Thermal effects in rapid directional solidification: Linear theory." 44th Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Tempe, AZ, 1992.

— Huntley, D. A., and Davis, S. H. "Thermal effects in rapid directional solidification." Tenth International Conference on Crystal Growth, San Diego, CA, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Evaluation of Microstructural Development in Undercooled Alloys*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 694-25-07-03

PRINCIPAL INVESTIGATOR: Dr. Richard N. Grugel
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TASK OBJECTIVE/DESCRIPTION

The objectives of this study are to be conducted in view of experiment and pertinent theory and will, upon completion, serve to enhance our scientific understanding of solidification processes. These include evaluating the microstructural morphology, external and internal to the sample, as functions of undercooling (ΔT), composition (C_o), and volume (V_o), Following microstructural evolution from the site of nucleation, this will provide valuable information with regard to maintaining the integrity of desired microstructure and the nature of abrupt morphological transitions. Irrefutable trends in microstructural development will be evaluated in terms of present theory, which will be amended as necessary. Finally, evaluation of the ground-based experiments will ascertain the feasibility of processing undercooled bulk melts in microgravity.

RESEARCH APPROACH

Nucleation of the undercooled alloy samples will be induced, and the extent of dendritic growth will be evaluated as a function of undercooling (C_o and V_o constant), composition (ΔT and V_o constant) and volume (T and C_o constant). Varying the composition will in effect vary the volume fraction of the primary dendrites and, consequently, the initial amount of heat released due to recalescence. Varying the sample size will affect the rate of cooling after recalescence.

Transitions in the microstructure, for example, a change from columnar dendritic to equiaxed grains, are also an important consideration and will be noted as a function of the above parameters. Critical evaluation of solute distribution and primary dendrite trunk diameters will provide information with regard to the internal dendrite growth velocity, and will allow for comparison with those measured on the sample surface. The internal solidification history will be further understood through evaluation of the evolution of the structure of interdendritic eutectic, and not merely the change in spacing.

PROGRESS DURING FY1992

Progress during 1992 year consisted primarily of equipment acquisition and incorporation into the laboratory, equipment characterization, development of experimental methods, and initiation of preliminary experiments.

A Lindberg Model 56724 furnace (max. temperature 1,700 °C) has been purchased and installed. The programmed heating and cooling rates have been measured by an independent thermocouple and found to be highly accurate; temperature stability is excellent.

Preliminary experiments with two alloy systems, Ag-14% Ge and Pb-30% Sn have been initiated. Ag-14 wt pct Ge: The primary silver phase has exhibited undercoolings on the order of 10 K and the eutectic has been undercooled 27 K. The solidified microstructures are in accordance with previous reports. A number of low-melting-point glasses are being evaluated as fluxes with the intent of achieving much greater undercoolings; "needles" to induce nucleation have been fabricated. Pb-30% Sn: The primary lead phase has been undercooled 11 K and the eutectic phase 22 K ($\Delta T/Tm = 0.12$). Microstructural examination shows a finer dendritic structure with increased undercooling, but for the given cooling conditions, no obvious macrosegregation.

Ms. Fay Hua, the graduate student assigned to this project, has done a through review of the relevant literature and is now familiar with alloy preparation, furnace operation, experimental procedures, and sample preparation for metallographic examination; her required class work is nearly completed.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Flanagan, W. F. "Microstructural development in bulk, undercooled alloys." Modular Containerless Processing Facility - Technical Interface Meeting, Jet Propulsion Laboratory, Pasadena, CA 13–15, January 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Noncontact Thermal, Physical Property Measurement of Multiphase Systems*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-25-07-04

PRINCIPAL INVESTIGATOR: Dr. Robert H. Hauge
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TASK OBJECTIVE/DESCRIPTION

Measurement methods for high-temperature materials in the liquid state are made difficult or impossible due to reactions with the support or container materials. Levitation methods (electromagnetic, electrostatic, aerodynamic, and acoustic) provide a containerless approach to sample positioning. Electromagnetic levitation also provides in situ heating and stirring of the sample. Our goal is to develop noncontact techniques of measurement for all relevant physical and chemical properties of the liquid state. Properties measurements which we are currently emphasizing are measurements of temperature, sample optical constant, density, surface tension, heat capacity, enthalpy, and thermal conductivity. The equipment allows for all of the above measurements to carry out of the same sample. Measurements of thermal conductivity are compromised by electromagnetic stirring forces and will require the quiescent environment of microgravity for accurate measurement.

RESEARCH APPROACH

Measurement techniques for the properties are as follows:

1. Temperature: A simultaneous measurement of sample brightness centered at 632 mm and the surface emissivity is made with an integrated multicolor pyrometer ellipsometer. This gives a noncontact measure of temperature with no assumptions. The surface refractive index and extinction coefficient are also obtained.

2. Density: A triggered high-resolution video camera image of the liquid drop is obtained with backlighting of the sample by a 670-mm diode laser. Images are taken when the sample has spherical symmetry, and the density is obtained from a calculation of volume with use of an accurately determined sample profile.

3. Surface tension: Surface-tension measurements are obtained from the vibrational frequencies of the oscillating drop. The vibrational frequencies are measured by following the fluctuation of reflected laser light.

4. Enthalpy and heat capacity: Drop calorimetry is currently used to measure the total sample heat content as a number of temperatures.

5. Thermal conductivity: Initial efforts are being made to determine the time-dependent temperature profile of a sample relative to spot heating with a CO_2 laser.

6. Electromagnetic levitation coils: Current concentrators which provide both vertical and lateral electromagnetic symmetry have been developed for efficient EM coupling to the sample and improved symmetry of the positioning forces.

PROGRESS DURING FY1992

New current concentrator designs have been shown to provide efficient electromagnetic (EM) coupling to the sample with symmetric positioning forces.

An integrated video camera, ellipsometer, and multicolor pyrometer instrument has been designed and is in a construction and testing phase.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Hauge, R. H., Lee, P., Baykara, T., and Margrave, J. L. A review of containerless thermophysical property measurements of liquid metals and alloys. Accepted by *High Temperature Science,* 1992.
— Krishnan, S., Nordine, P. C., Weber, J. K. R., Hauge, R. H., and Margrave, J. L. Emissivity and temperature measurement by laser polarimetry and spectoral radiometry. *Proceedings of the Seventh International Symposium on Temperature, May 1, 1992.*
— Xiao, Z. L., Lee, P., Fredin, L., Hauge, R. H., Margrave, J. L. Methods development for sample size, thermodynamic temperature, surface tension and motion measurements of levitated samples. The Gordon Research Conference (High Temperature Chemistry), July 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: ***Fluid Flow in Partly Solidified Systems***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-19

PRINCIPAL INVESTIGATOR: Prof. Angus Hellawell
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TASK OBJECTIVE/DESCRIPTION

This research is concerned with the occurrence of local macroscopic convective patterns which develop in bulk liquids during alloy solidification and lead to segregation in the solidified material. Thermosolutal plumes are interesting scientifically because they represent a convective stability problem, and industrially because their occurrence in metal casting causes the defect known as "frackle."

RESEARCH APPROACH

We propose to carry out studies of channel formulation in molten salts (NaF-NaC1) and organics (SCN). We intend to correlate the thermal, compositional, and dimensional conditions for channel formation in the salts and organics and compare the results with those already available for lead-based alloys and the aqueous system.

PROGRESS DURING FY1992

During the year the techniques have been refined for measurements of channel-convective plume dimensions, compositions, and flow rates, for metallic, aqueous, and organic systems, covering a range of Prandti numbers from ~2.10E-2 to ~20. With refined optical techniques and with video recording at 1/30s frame intervals, considerable data is now becoming available about the movement and density distribution of small dendrite fragments which are ejected from the mushy zone into the bulk liquid.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Hellawell, A., Sarazin, J. R., and Steube, R. S. Channel convection in partly solidified systems. In preparation, 1991.
— Jang, J., and Hellawell, A. The use of NH_4Cl-H_2O analogue castings to model aspects of continuous casting, Parts I and II. *J. Ironmaking and Steelmaking.*, vol. 18, pp. 267–283, (1991)

— Sarazin, J. H., and Hellawell, A. Segregation arising from natural convection during solidification. *TMS, EPD Congress Proceedings*. D. R. Gaskell, ed., pp. 511–522, 1992.

— Steube, R. S. , Sarazin, J. H., and Hellawell, A. "Observations of convection during solidifcation." TMS Spring Meeting, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Containerless Processing of Oxide Superconductors*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-25-08-22

PRINCIPAL INVESTIGATOR: Dr. William H. Hofmeister
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TASK OBJECTIVE/DESCRIPTION

The high reactivity of oxide superconductors with all known containing media makes them excellent candidates for containerless processing experiments. $YBa_2Cu_3O_{7-\delta}$ or 1:2:3 has been chosen as the prototype material for these studies because the phase relationships are reasonably well known and, as this is a peritectic compound, the possibility of solidifying if directly from an undercooled melt is reasonably high.

The experimental objectives are to develop viable techniques for containerless processing of oxide superconductors, to explore the melting, undercooling, and solidification behavior of these materials, and to study the microstructural and superconducting properties of the resultant materials. Comparison of these melt-processed materials with ceramic, melt-textured, and directionally solidified materials will help to elucidate the advantages and disadvantages of containerless processing on oxide superconductors. The techniques developed by this project will apply to oxide superconductors in general and will provide additional avenues for research in this field.

RESEARCH APPROACH

Containerless processing will be performed using a 2-meter drop tube and powders of starting composition $YBa_2Cu_3O_{7-\delta}$ ranging in size from 10 cm to 300 cm. This drop tube allows for processing in a controlled environment free from container contamination.

Microstructural and compositional analyses will be performed by both Vanderbilt and Westinghouse. In addition, other methods of containerless processing will be explored including aero-acoustic levitation, electrostatic levitation, and cold-crucible electromagnetic levitation.

PROGRESS DURING FY1992

Powders have been processed in the 2-meter drop tube at Vanderbilt at temperatures up to 1,750 °C. Microstructural evaluation involved optical microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Resultant phases were characterized by X-ray diffraction (XRD), energy dispersive spectroscopy (EDS), and electron diffraction.

The microstructures consisted of faceted Y_2O_3 particles from 1-3 cm in size surrounded by at least three other phases including a previously unreported hexagonal phase with composition $YBa_2Cu_{3.5}O_x$. The nature of the Y_2O_3 particles indicates that complete melting did not take place in experiments with furnace temperatures below 1,720 °C. At higher furnace temperatures complete melting followed by undercooling, and rapid solidification did occur. This was evidenced by a duplex microstructure, typical of metals that have been undercooled and rapidly solidified. The rapidly solidified region had an overall composition of approximately 1:1:1.8 and consisted of submicron Y_2O_3 particles surrounded by an extremely fine matrix of several phases, most of which were nanoscale. Throughout all of these drop-tube experiments, variation of the oxygen content in the processing environment appeared to have no effect on the resulting microstructure.

In an effort to determine the exact location of the Y_2O_3 liquidus in this system, experiments were performed using compounds of stoichiometry 1:1:2 and 1:2.4:3.2. In both cases, complete melting did not occur; however, some insight was gained as to the origin of several of the phases. In addition to the drop-tube experiments performed, investigations have been initiated into aero-acoustic levitation (AAL) using the facility at Intersonics, Inc. in Chicago, IL. This technique provides several advantages over the 2-meter drop tube. Samples range in size from 2 to 3 mm, thus greatly simplifying the metallography and making it easier to characterize the microstructures. AAL also allows for direct observation of the sample while processing. This provides both a visual record of melting and solidification as well as accurate temperature measurement. In addition, much higher temperatures are attainable with AAL. This should help to overcome the temperature limitations of the 2-meter drop tube, allowing access to the Y_2O_3 liquids.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Olive, J. R., Hofmeister, W. H., Carro, G., and Bayuzick R. J. "Containerless processing of oxide superconductors." Vanderbilt University, Nashville, TN, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Modeling/Experimental Studies of Droplet Pushing in Miscibility-Gap Alloy Solidification Under Low-g Conditions*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-22

PRINCIPAL INVESTIGATOR: Dr. William B. Krantz
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TASK OBJECTIVE/DESCRIPTION

The focus of this study is to understand the mechanism of droplet rejection by an advancing solidification front during directional solidification of a miscibility-gap alloy. The droplet-pushing phenomenon is thought to be an important factor governing the formation of microstructures in these alloys.

RESEARCH APPROACH

The first objective of this research is to obtain qualitative and quantitative information on the droplet-pushing mechanism by observation of the solidification front in transparent organic miscibility-gap systems.

The second objective is to develop a mathematical model of droplet pushing which predicts the critical drop diameter as a function of processing conditions and fluid properties. The final objective is to determine the proper form of the thin film model for the droplet-pushing problem.

PROGRESS DURING FY1992

Progress has been made in experimental and modeling studies. The difficulties encountered with achieving and maintaining high sample purity prompted the development of a system for purification and transfer of organic materials. Solidification experiments suggested that the critical drop size was dependent on the shape of the solidification front. A numerical solution for the critical drop site was developed which treats the solidification front as a free boundary. Progress on thin film modeling includes the identification of a continuum film pressure tensor.

GRADUATE STUDENTS: 5 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Chione, D. J., Wray, M. D., Thiessen, D. B., and Krantz, W. B. "Surface tension measurement by digital image analysis." Southwesstern and Rocky Mountain Division of the American Association for the Advancement of Science, 68th Annual Meeting, Tuscon, AZ, May 17–21, 1992.

— Thiessen, D. B., and Krantz, W. B. Bimodal terminal velocities using the falling needle viscometer. *Rev. Sci. Instrum.* In press, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Containerless Property Measurement of High-Temperature Liquids*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 694-25-07-05

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TASK OBJECTIVE/DESCRIPTION

The task objective is to measure the optical properties of high-purity liquid metals and alloys (Al, Zr, Ni, and Ni-Zr alloys) over wide wavelength (220–1100 nm), temperature (Tm,l + 300 K), and composition ranges under containerless conditions. Spectroscopic, pulsed dye-laser ellipsometry is used to obtain the complex dielectric functions and spectral emissivity data at high temperatures on clean liquids using electromagnetic levitation. These data are needed for accurate noncontact temperature measurement, and for measurements of the total hemispherical emittance by integration of emissivity over the wavelength range of thermal emission.

The relevance and significance to the microgravity program are twofold. First, the spectral emissivity and total hemispherical emissivity form the basis for new noncontact thermophysical property measurements in microgravity experimentation. For example, knowledge of total hemispherical emittance allows heat capacity and thermal diffusivity to be accurately determined from free-cooling and pulse-heating experiments. Spectral emissivity data allow true specimen temperatures to be determined using optical pyrometry. Second, spectral emissivity measurements on specific materials are needed by other NASA investigators in ground-based and microgravity experimentation.

Another major outcome of this research will be the determination of the optical properties of liquids over a wide wavelength range. These measurements are of fundamental importance to advancing the theory of liquid metals. For example the presence or absence of important interband transitions provides information on the valence, bonding, joint density-of-states, and the extent to which nearly-free electron behavior is exhibited by liquid metals and alloys.

RESEARCH APPROACH

The research approach is to levitate liquid metals and alloys (Al, Ni, Zr, and Ni-Zr alloys) electromagnetically and use a spectroscopic pulsed dye-laser ellipsometer to

measure the complex dielectric function and the spectral emissivity in the wavelength range 220--100 nm. Pulsed radiation is generated by a Molectron dye-laser, and the wavelength is automatically set and adjusted by a laboratory computer. Light reflected by the specimen is collected and analyzed by a unique rotating analyzer ellipsometer.

The rotating components of the ellipsometer are motorized and controlled by the computer. The signals are detected by a pair of photodiodes and an EG&G boxcar averager is used to extract the mean value of the light intensities at the two photodiodes which receive the orthogonally polarized components of the reflected light. The signals are automatically measured by the computer.

A Molectron dye laser is used to generate pulsed radiation in the 220–1100 nm wavelength range. The light is steered through several mirrors, and transmitted through a pair of Glan Thomson linear polarizers. The second polarizer is fixed in azimuth, and rotation of the first polarizer allows light levels to be adjusted to the optimum values. The light is incident on the liquid specimens at a fixed incident polarization, and the reflected polarization is analyzed for its new azimuth and ellipticity.

A modified rotating analyzer ellipsometer is used to measure the outgoing polarization at 6 azimuths of the analyzer. The analyzer is of the beamsplitting type such that the two orthogonal components of the beam are simultaneously obtained. Three intensity ratios are measured at three independent pairs of azimuths. The complex dielectric constant, indices of refraction, and spectral emissivities are derived from standard equations. The light intensities are detected by a pair of high speed, UV-enhanced silicon photodiodes and measured by a pair of gated integrators.

The emphasis of measurements on liquid metals and alloys is to determine the temperature and (for alloys) composition dependence of all optical properties over the accessible wavelength range. Measurements are possible from approximately 0.8 of the melting temperature, (TM) in undercooled liquids to at least 300K above TM. The observed effects of temperature and composition on optical properties and the wavelength dependence of these properties are interpreted in terms of liquid structure and bonding.

The liquid nickel, zirconium, and their alloys have been chosen to be investigated in this research because they display unique glass forming behavior, typify early and late transition metals, and because they are also of interest to other NASA investigators. Measurements at 633 nm on these metals is being conducted in collaboration with Professors Bayuzick of Vanderbilt University and Johnson of the California Institute of Techology.

PROGRESS DURING FY1992

An automated rotating analyzer pulsed dye laser spectroscopic ellipsometer was designed and built during the first three months of the project. It consists of a nitrogen laser-pumped pulsed dye laser and a rotating analyzer polarization state detector (PSD). The incident laser beam and PSD axes are placed at an angle of 135° in the horizontal plane and perpendicular to two windows on the electromagnetic levitation chamber. Specimens are levitated and melted at the intersection of these axes, using specially designed levitation coils that do not obscure the equatorial plane of the levitated drop. Incident laser light of a fixed polarization state is reflected into the PSD and analyzed. The PSD includes light collection and focusing optics, a beam splitting Glan-Thompson prism mounted in a computer-operated rotation stage, and a pair of photodiodes.

The new apparatus was successfully used to determine the optical properties of liquid aluminum at wavelengths from 360,990 nm (1.2–3.5 eV) at a temperature of 1,580 K. Data at eight wavelengths were obtained over the temperature range from 1,200 K–1,800 K. Structure in the optical properties of liquid aluminum was demonstrated to occur at photon energies of ca. 1.5 eV (820 nm wavelength). This is the first demonstration that liquid aluminum has structure in the optical properties and displays the nonfree electron behavior characteristic of solid aluminum. Error analyses have been conducted to establish the accuracy of results. Further analysis of the results is in progress and a paper on this work is being prepared for publication. Experiments are in progress to develop electromagnetic levitation coils and conditions for measurements on liquid zirconium and nickel.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Krishnan, S., Calibration, properties and applications of the division-of- amplitude photopolarimeter at 632.8 and 1523 nm. *J. Opt. Soc. Am. A ,9*, 1615–1622 (1992).

— S. Krishnan and P. C. Nordine, Containerless property measurements of high temperature liquids: emissivity, temperature, thermodynamics, In *Proceedings of the First Technical Interface Meeting for the Modular Containerless Processing Facility*, Jet Propulsion Laboratory Publication JPL D-9370, 1992.

— Krishnan, S. and Nordine, P. C., Optical properties of clean liquid aluminum at 1.2 - 3.6 eV. For *Phys. Rev. B.* In preparation, 1992.

— Krishnan, S., Weber, J. K. R., Anderson, C. D., Nordine, P. C., and Sheldon, R. I. "Optical properties of liquid uranium and zirconium at 633 nm." Presented at the Gordon Research Conference on High Temperature Chemistry, Meriden, NH, July 19–24, 1992.

— Krishnan, S., Weber, J. K. R., Anderson, C.D., Nordine, P. C., and Sheldon, R. I. Spectral emissivity and optical properties at A = 632.8 nm for liquid uranium and zirconium at high temperatures. *J. Nucl. Matter.* Submitted for publication, 1992.

— Krishnan, S., Nordine, P. C., Weber, J. K. R., Hauge, R. H., and Margrave, J. L. Emissivity and temperature measurement by laser polarimetry and spectral radiometry. In J. F. Schooley, ed., *Temperature its Measurement and Control in Science and Industry*, vol. 6, part 2. New York: American Institute of Physics, pp. 943-948 (1992).

— Krishnan, S., Anderson, C.D., Weber, J.K.R., Nordine, P.C., Hofmeister, W.H., and Bayuzick, R. J. Optical properties. *Metall. Trans A*, December 1992 (in press).

— Krishnan, S., Nordine, P. C., Weber, J. K. R., Hauge, R. H., and Margrave, J. L. "Emissivity and temperature measurement by laser polarimetry and spectral radiometry." Presented at the 7th Symposium on Temperature, Toronto, April 28 – May 1, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Containerless Processing for Controlled Solidification Microstructures*
RESPONSIBLE CENTER: LeRC PROJECT IDENTIFICATION: 694-25-07-06

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TASK OBJECTIVE/DESCRIPTION

The main research objective is the evaluation of the undercooling and resultant solidification microstructures in containerless processing, including drop-tube processing and levitation melting of selected alloys as an experience base for microgravity experiments.

RESEARCH APPROACH

The degree of liquid undercooling attainable in a laboratory scale (3-m) drop-tube and levitation melting system can be altered through the variation of processing parameters such as melt superheat, sample-size, and gas environment. In a given sample, the competitive nucleation and growth kinetics between equilibrium and metastable phases controls microstructural development. The solidification behavior is evaluated through metallography, thermal analysis, and X-ray diffraction examination in conjunction with calorimetric measurements of falling droplets and a heat flow model of the processing conditions to judge the sample thermal history.

PROGRESS DURING FY1992

In the current program studies, solidification microstructures are being examined in selected Ni- and Mn-based systems. The specific alloy selection is based on a metastable phase diagram analysis that allows for the identification of unique microstructures and microstructural transitions that may be produced by microgravity containerless processing.

A duplex partitionless solidification reaction involving fcc and bcc crystalline phases has been identified over a range of compositions near that of the eutectic in the Ni-V system. The reaction can be thought of as the limiting case of a eutectic transformation ($L \rightarrow \alpha + \beta$) in which α and β have the same composition as the liquid phase. Drop tube experiments are being conducted to characterize the competitive formation kinetics of the fcc and bcc phases. Near-equiatomic Ni-V alloys were

solidified via containerless processing methods and studied with electron microscopy techniques. TEM has shown the presence of a duplex structure of fcc and bcc in large (≈100 mg) droplet samples. Microstructural analysis has suggested that the duplex structure is not the result of a solid state transformation and that the fcc and bcc phases have apparently nucleated independently from the liquid phase.

A thermodynamic model has been applied to the Ni-V system to calculate T_0 temperatures for the relevant phases to map compositions and temperatures for which the duplex partitionless reaction is possible. A kinetic model has also been forwarded, which takes into account both the nucleation and growth rates of the competing fcc and bcc phases. The nucleation kinetics analysis is in agreement with experimental results. Further refinement of the model is underway to consider the effects of transient nucleation and heat flow effects.

Near-equiatomic Mn-AI alloys represent an important class of permanent magnet materials. The key ferromagnetic phase is a metastable structure produced by solid-state heat treatments. Recent drop-tube and levitation melting studies have demonstrated for the first time that the metastable ferromagnetic phase can be produced from the liquid, provided that high undercooling is achieved. With specially prepared samples, it has been possible to assess the thermodynamic driving forces involved in metastable τ phase solidification. The T_0 τ/l temperature has been evaluated to help understand the metastable solidification reaction pathways which yield the ferromagnetic τ phase during the containerless processing.

Building on the thermodynamic analysis, a competitive nucleation model has been developed to account for the observed phase selection. As part of a test of the kinetics model a detailed statistical study of the metastable product yield as a function of sample size and of processing gases, such as He and Ar gases, is underway. Furthermore, by optimizing the containerless processing conditions in levitation melting it has been possible to obtain essentially single-phase samples of the I structure for sample-size scale up (mm size) to approach bulk levels. In the above studies a new calorimetric system is being used to measure the temperature of falling drops during containerless processing to assess the complete thermal history.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 1

PUBLICATIONS/PRESENTATIONS

— Allen, D. R., Das, S., and Perepezko, J. H. Kinetic competition during duplex partitionless crystallization. *Journal of Non-Crystalline Solids* in press, 1992.

— Allen, D. R., and Perepezko, J. H. "Kinetic competition during duplex partitionless crystallization." Fourth International Symposium on Nucleation and Crystallization in Liquids and Glasses, Stone Mountain, GA, August 1992, and TMS/ASM Fall Meeting, Chicago, IL, November 1992.

— Yong, J. K., and Perepezko, J. H. The thermodynamics and competitive kinetics of metastable τ phase development in MnAl-base alloys. *Materials Science and Engineering* in press, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *The Role of Gravity in Macrosegregation in Alloys*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 674-25-05-17

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TASK OBJECTIVE/DESCRIPTION

The major objective is to develop comprehensive convection/solidification computer codes to model macrosegregation in alloys that freeze in a dendritic mode. The finished codes could be used to design experiment to study the effect of a low-gravity environment on macrosegregation in binary alloys. It is also anticipated that the codes would be used to assist engineers in designing or controlling commercial casting processes in which convection is driven by gravity.

RESEARCH APPROACH

In order to model macrosegregation phenomena in alloys which freeze dendritically, a quantitative analysis of solute redistribution is absolutely necessary. Hence appropriate forms of the mass, momentum, and energy equations must be selected to predict each of these transport processes in solidifying castings.

In addition to predicting macrosegregation variation is across a casting or from its bottom to top, major emphasis is on modeling the intricate convective phenomena responsible for localized defects, often called "freckles," which are particularly troublesome to practioners. Emphasis is on multidiffusive convection, which is thought to be the cause of the "freckles." When combined with thermodynamic data for gas-forming reactions, the basic solidification model can be extended to predict the conditions when interdendritic porosity forms or, indeed, to predict the avoidance of such a defect. Because the overall program deals with defectavoidance, it is expected that practitioners will derive significant benefit from the research.

PROGRESS DURING FY1992

A part of the early effort in the program was in collecting and evaluating physical and thermal properties. Such data must be quantitatively analyzed so that extrapolation to the solidification temperature range can be made with confidence.

Linear stability analyses and nonlinear calculations for a fully convecting system were done for a liquid layer above a stationary porous medium with constant

porosity for both isotropic and anisotropic media. The model was also extended to treat alloy solidification more realistically by considering an all-liquid zone above a mushy zone moving with a prescribed solidification velocity and with a variable volume fractionof liquid in the mushy zone that is consistent with solidification thermodynamics. Linear stability analyses were done in order to define marginal stability curves for the onset of convection in Pb-20 wt % Sn alloys, in terms of thermal gradient versus the horizontal wave number at various gravitional constants. Calculations of the nonlinear convection were also done. These calculations verified the linear stability calculations and showed that, when there is convection, flow in the upper part of the mushy zone is driven by the convection in all-liquid region.

Another accomplishment was the development of a code to treat steady-state directional solidification of a binary alloy in the form of a circular cylinder. The code can be used to examine the sensitivity of the interdendritic convection and macrosegregation to a slight curvature of the nominally horizontally isotherms in the mushy zone of a DS casting.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Electrostatic Containerless Processing*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-25-04-08

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TASK OBJECTIVE/DESCRIPTION

The Electrostatic Containerless Processing Task objective is to utilize the advanced capabilities provided by the electrostatic positioner for the investigation of thermophysical properties of undercooled molten metals and alloys, various nucleation kinetics, and of the possibility of creating metastable phases, thus giving access to a whole range of materials with novel properties.

RESEARCH APPROACH

Metallic samples about 3 mm in size are levitated in vacuum in a very quiescent state and superheating-undercooling-recalescence cycles are repeated. This high-temperature electrostatic levitator has the following important capabilities: (a) it provides quiescent and clean processing environment without inducing flows or contaminating the sample, (b) both conducting (metals or alloys) and nonconducting (semiconductors or ceramics) materials can be processed, (c) sample temperature can be independently controlled without interfering levitation force, and (d) it provides wide open sample viewing for various diagnostic instruments.

PROGRESS DURING FY1992

There has been a significant breakthrough in high-temperature electrostatic levitation technology in 1992. The basic capabilities of melting and solidification during levitation have been verified using various high-density materials, such as: In (T_m=157 °C), Sn (232 °C), Bi (271.44 °C), Pb (327 °C), In (0.69%) Sb (492.5 °C), Al (670 °C), Ge (938 °C), Cu (1083 °C), Ni (1,455 °C), and Zr (1,855 °C).

This preliminary work was followed by an extensive undercooling-nucleation study jointly with Vanderbilt University. Using two zirconium samples of different origin and purity, over 300 runs of superheating-undercooling-recalescence processes have been completed. A patent application is in progress for the high-temperature electrostatic levitator of Won-Kyu Rhim and Sang K. Chung.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Rhim W. K. and Chung S. K. Characteristic oscillation of rotating drops. In preparation, 1992.
— Rhim, W-K., and Chung, S-K. The high-temperature electrostatic levitator. New Technology Report, 1992.
— Rhim, W-K., Chung, S-K., Barber, D., Man, K. F., Gutt, G., Rulison, A., and Spjut, R. E. A high-temperature electrostatic levitator for the containerless processing of metals and alloys. In preparation, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Crystal Nucleation, Hydrostatic Tension, & Diffusion in Metal Melts*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** 694-25-07-07

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TASK OBJECTIVE/DESCRIPTION

The objective is to develop basic understanding of the phenomena and processes that are central to the microgravity program: crystal nucleating, glass formation, and diffusion in the liquid state.

RESEARCH APPROACH

Crystal nucleation is studied in elemental metal, semiconductor, or quasi-crystal-forming droplets coated with different fluxes, droplets with clean surfaces in vacuum, and droplets solidified in a drop tube. The effect of hydrostatic stress on the nucleation kinetics is studied by dilatometry. The crystal-melt interfacial tension is studied experimentally and theoretically, The diffusivity in the liquid state is measured from the broadening of impurity profiles after pulsed laser melting.

PROGRESS DURING FY1992

Work on the present task has been going on for only nine months, with the following progress.

• David T. Wu has made important new contributions to the analysis of multicomponent nucleation and the associated time lag, as well as to a problem that is formally very closely related to it: the kinetics of chain reactions.

• Undercooling of silicon droplets has been attempted in various oxide and halogen fluxes. The problems with oxide fluxes, observed in preliminary work by Devaud and Turnbull, were confirmed. It is hoped that the use of chloride or fluoride fluxes will be more successful for the removal of nucleants.

• Dilatometry work on crystal nucleation in oxide-coated Ga droplets has started. Preliminary experiments show a complicated behavior that requires further analysis.

• Drop-tube experiments on Al-Cu-Fe and Al-Pd-Mn quasi-crystal-forming melts are underway, in collaboration with A.L. Greer at the University of Cambridge (UK).

In addition, the diffusivities of Fe and Cu in liquid Al were measured by melting thin Al films with a nanosecond-duration pulsed laser. The thin-film geometry eliminated convection in the melt during the experiment and simplified the measurement of the diffusion coefficient in liquid. The transition conductance and the optical reflectance of the Al layer during melting were measured to obtain the melt duration. The diffusivity of Fe was found to be much smaller than that of Cu, which is consistent with Turnbull's proposal of cluster formation in Fe-Al melts as an explanation of their volumetric behavior.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Nobuaki I., Smith, P. M., and Aziz, P. M. Anomalous diffusion of Fe in liquid Al. In preparation, to be submitted to *Acta Metallurgica et Materialla,* 1992.

— Spaepen, F. A. Fundamentals of nucleation and growth.*Optical Data Storage, Proceedings of SPIE-The International Society for Optical Engineering,* Bellingham, WA, *1663,* 385–386 (1992).

— Wu, D. T., and Aziz, M. J. The kinetics of chain reactions: Implications for solid phase epitaxy. In preparation, to be submitted to *Journal of Applied Physics,* 1992.

— Wu, D. T. The time lag in mult-component nucleation. In preparation, to be submitted to *Journal of Chemical Physics.,* 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Levitation Undercooling Nucleation*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** 674-25-04-09

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TASK OBJECTIVE/DESCRIPTION

The principal objectives of this task are to utilize containerless manipulation technology to perform (a) undercooling and heterogeneous nucleation experiments on pure metals and alloys as well as organic and inorganic model materials, (b) measurement of the physical properties of undercooled melts, and (c) investigation of undercooled and solidification of phase-separated model materials and eutectic alloys.

RESEARCH APPROACH

The research approach is to use ground-based ultrasonic and electromagnetic levitation techniques, together with novel noncontact property measurement methods, to undercool millimeter-size samples in a containerless manner; to characterize the levitation environment to determine possible "dynamic" nucleating effects; and to develop limited theories to investigate specific alloy systems.

PROGRESS DURING FY1992

FY1992 research tasks have included (a) the measurement of the specific heat of Ti-Cr alloys in stable and undercooled liquid ranges, (b) the initiation of the thermal diffusivity measurement of levitated melts, and (c) the initiation of a total hemispherical emissivity measurement task using electromagnetically levitated samples.

FY1993 tasks will include (a) the continuation of the total hemispherical emissivity measurement, (b) the studies of undercooling using electromagnetically leviated melts of Al-Cu alloys in comparison with electrostatically levitated samples to uncover possible "dynamic" effects on nucleation, and (c) the initiation of the experimental study of ultrasonically levitated phase-separated model materials (aqueous solutions of succinonitrile).

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Ohsaka, K., Gatewood, J. R., and Trinh, E. H. An apparatus for the specific measurement of undercooled liquids. *Scripta Metallurgica et Materiala, 25,* 1459, (1991).

— Ohsaka, K., Holzer, J. C., Trinh, E. H., and Johnson, W. L. Specific heat measurement of undercooled liquids. *Proc. of Exp. Methods for Microgravity Materials Science Research 4th Int. Symposium*. R. A. Schiffman, ed., p. 1, TMS 1992.

— Ohsaka, K., Trinh, E. H., Holzer, J. C., and Johnson, W. L. The Gibbs free-energy difference between the undercooled liquid and the B phase of a Ti-Cr alloy. *Appl. Phys. Lett., 60,* 1079 (1992).

— Sadhal, S., Trinh, E. H., and Wagner, P. "Unsteady spot heating of a drop in a microgravity environment." ASME winter annual meeting, Anaheim, California, 1992.

PATENTS

— Trinh, E.H., and Gaspar, M. "Method for Controlled Sample Rotation in a Single-axis Acoustic Levitator." US Patent 4,777,823.

— Trinh, E.H. and Robey, J.L. "Acoustic Convective Cooling/Heating Device for Microgravity." US Patent 4,856,717.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Coarsening of Solid-Liquid Mixtures*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-25-08-21

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TASK OBJECTIVE/DESCRIPTION

The late stages of a first-order phase transformation process are usually characterized by the growth of second-phase domains with low interfacial curvature at the expense of domains with high interfacial curvature. This process, also known as Ostwald ripening or coarsening, occurs in a wide variety of two-phase mixtures ranging from multiphase solids to multiphase liquids, and has a significant impact on the high-temperature stability of many technologically important materials. Unfortunately, an understanding of the dynamics of ripening processes is not in hand. Many of the recent theories for the effects of a finite volume fraction of coarsening phase on the kinetics of Ostwald ripening have proposed divergent expressions for the dependence of the coarsening rate of the system on the volume fraction of coarsening phase. As there are virtually no experimental data of sufficient quality to differentiate between these theories, the controversy over the dependence of the coarsening rate of the system on the volume fraction remains unresolved.

Previous NASA-sponsored work clearly showed that solid-liquid mixtures consisting of Sn-rich particles in a Pb-Sn eutectic liquid are ideal, and perhaps unique, systems in which to explore the dynamics of the Ostwald ripening process. The high coarsening rate in these systems permits accurate kinetic data to be obtained, and the thermophysical parameters necessary to make a comparison between theory and experiment are known. However, in a terrestrial environment experiments can be performed only at the relatively high-volume fractions of solid, where the presence of a solid skeletal structure prevents large-scale particle sedimentation.

In these high-volume fraction experiments, a comparison between theory and experiment shows that the solid-liquid mixtures are coarsening faster than predicted by an approximate theory for purely diffusional controlled Ostwald ripening. The objective of this project is to plan and perform a microgravity experiment on Ostwald ripening in solid-liquid mixtures. This experiment will serve two primary

purposes: it will allow experiments to be performed which can be directly compared to heretofore untested theories for coarsening in systems with low-volume fractions of solid, and it will eliminate conclusively convection of the liquid matrix and small-scale particle motion within the skeletal structure as possible sources for the disagreement observed between theory and experiment in the high-volume fraction experiments.

RESEARCH APPROACH

Concurrent with our work on designing a spaceflight experiment, ground-based experimental and theoretical studies on Ostwald ripening will be undertaken in an effort to provide comparison experiments to those performed in microgravity and to provide a theoretical understanding of the Ostwald ripening process.

We are thus investigating the nature of transient Ostwald ripening in solid-liquid systems and developing a first-principles theory for ripening in systems with volume fractions of coarsening phase above 0.1. Such volume fractions are closer to those employed in the ground-based experiments and will permit theory to be compared with the results of the spaceflight experiments over a wider range of volume fractions than is currently possible. Finally, the transient Ostwald ripening experiments will allow us to determine the time required for the spacefight experiment.

PROGRESS DURING FY1992

We have examined theoretically the time-dependent behavior of a two-phase system undergoing transient Ostwald ripening. The evolution of selected initial particle-radius-distribution (prd) functions was followed to over three orders of magnitude in time. Although steady-state coarsening behavior was never fully achieved, the existence of the Lifshitz-Slyozov (LS) attractor prd and scaling laws for r and N_v was essentially confirmed for systems with zero volume fraction of coarsening phase and a wide range of initial PRD's.

The transition path to steady-state coarsening was highly dependent upon the initial PRD. Phase-plane plots illustrated this independence and showed the large basin of attraction for the LS prd. In addition, changes in the initial form of a given prd within a fixed class of prd's were found to affect strongly the transient coarsening rate; for example, wide log-normal prd's evloved more rapidly than did narrow ones. Calculations were also done to examine the effect of a finite volume fraction of coarsening phase on the extent of the transient regime. The results showed that the system evolved to its steady-state form more rapidly at nonzero volume fraction than at zero volume fraction.

In addition, we have developed a method for solving a multiparticle diffusion problem which can be used to describe the ripening process in systems with a high volume fraction of coarsening phase. Large-scale numerical simulations of the coarsening process were performed using this description of the diffusion field in

an effort to determine the statistically averaged properties of coarsening ensembles. We find that at volume fractions as low as 0.1 particles are not distributed randomly in space.

We have measured spatial correlation functions between particles of various sizes. These results show that large particles tend to be surrounded by small particles during coarsening, but the extent of this clustering is a strong function of the volume fraction of coarsening phase. At volume fractions above 0.1 we find that the centers of mass of the particles can move via a solution-reprecipitation process and that rate constants determined from the simulations are greater than those found in previous simulations that employed a more approximate solution to the diffusion equation.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Akaiwa, N. "Effects of a large volume fraction of coursening phase on the kinetics of Ostwald ripening." TMS annual meeting, San Diego, CA, March 1992.

— Akaiwa, N., Hardy S. C., and Voorhees, P. W., The effects of convection on Ostwald ripening in solid-liquid mixtures. *Acta Met. Mater.* , *39*, 2931, (1991).

— Chen, M. "The dynamics of transient Ostwald ripening." TMS annual meeting, San Diego, CA, March 1992.

— Hardy, S.C., McFadden, G.B., Coriell, S.R.,Voorhees, P.W. and Sekerka, R.F. Measurement and analysis of grain boundary grooving by volume diffusion. *J. Cryst. Growth* , *114*, 467 (1991).

— Voorhees, P. W., "Ostwald ripening in two-phase mixtures: Beyond mean field theory." Invited address, TME fall meeting, Chicago, IL, October, 1992.

TYPE: Ground
DISCIPLINE: Metals and Alloys
PROJECT TITLE: *Influence of Convection on Microstructure*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-25-08-17

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TASK OBJECTIVE/DESCRIPTION

The objective of this research is to gain an understanding of the influence of gravity on the microstructure of eutectics, especially MnBi-Bi. Research tasks were established to determine:

1. Via theoretical calculations, the influence of convection on the microstructure of fibrous eutectics;

2. Via theoretical calculations, the influence of the Soret effect (thermal diffusion) on eutectic microstructure;

3. An estimate of the Soret coefficient of eutectic MnBi-Bi melts, using laboratory data and data from the flight experiment of Dr. David Larson at Grumman;

4. Via theoretical calculations, the influence of convection on eutectic microstructure when one phase projects out into the melt ahead of the other phase;

5. Experimentally, the influence of vibration during solidification on eutectic microstructure;

6. Experimentally, the influence of centrifugation during solidification on eutectic microstructure; and

7. Experimentally, the influence of deviations from eutectic composition on the microstructure of directionally solidified MnBi-Bi.

RESEARCH APPROACH

The research involved two approaches:

1. Directional solidification of Mn-Bi and Pb-Sn alloys and then the determination of microstructure;

2. The numerical calculation of concentration field in front of growing interface, and then the determination of microstructure for minimum undercooling.

PROGRESS DURING FY1992

Prior to this fiscal year we completed tasks 1–5, except that the estimate in task 5 does not include data from Dr. Larson.

Task 6 has been delayed. We had originally hoped to perform experiments in centrifuges in Canada and France, but this turned out to be impractical, and so we are constructing our own centrifuge facility here. We expect to begin doing experiments on the Mn-Bi system in early 1993. Task 7 is nearly complete.

GRADUATE STUDENTS: 3 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Caram, R., and Wilcox, W. R. "Analysis of thermotransport during rod eutectic solidification." First International Conference on Transport Phenomena in Processing, Honolulu, HI, March 1992.

— Caram, R., and Wilcox, W. R. The Soret effect in eutectic solidification *J. Mat. Proc. & Manuf. Sci.*, *1*, 56–68 (1992).

— Caram, R., Banan, M., and Wilcox, W. R. Directional solidification of Pb-Sn eutectic with vibration. *J. Crystal Growth, 114*, 249–254 (1991).

— Rydzewski, J. H., and Wilcox, W. R. Influence of gravity on the microstructure of the MnBi/Bi eutectic. INternational Astronautical Federation Congress, Montreal, Quebec, Canada, October 1991. *Acta Astronautica* (in press), 1992.

— Seth, J. S., and Wilcox, W. R. Effect of convection on the microstructure of a lamellar eutectic growing with a stepped interface. *J. Crystal Growth, 114*, 357–363 (1991).

— Rydzewski, J. H., and Wilcox, W. R. "Influence of gravity on the microstructure of the MnBi/Bi eutectic." International Astronautical Federation Congress, Montreal, Quebec, Canada, October 1991.

TYPE: Ground
DISCIPLINE: Protein Crystal Growth
PROJECT TITLE: *Crystallographic Studies of Proteins*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-23-08-17

PRINCIPAL INVESTIGATOR: Dr. Daniel C. Carter
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TASK OBJECTIVE/DESCRIPTION

The objectives of this research are to: (a) determine and refine the structure of human serum albumin (HSA) to 3.0 angstroms resolution; (b) determine and refine the structure of a novel fungal lysozyme from *Chalaropsis*; (c) determine and refine the high resolution of the oxidized and reduced forms of cytochrome c5 from *Azotobacter*; and (d) evaluate the effects of microgravity on the growth of selected protein crystals. This proposal is concerned with basic research support for several in-house protein structural problems, and for the capabilities expansion of, and support for, the existing diffraction facility.

The three primary protein structural problems which are being studied at Marshall Space Flight Center, some aspects of which include flight experiments, have been synopsized on the following pages of this summary. These projects include the characterization and structure determination of HSA, AIDS antibody structure, *Chalaropsis* lysozyme, and the high-resolution structure determination of the electron transport protein cytochrome c5. It is anticipated that the further development of this facility, and the successful completion of selected aspects of this research, will have a significant impact on the scientific—as well as on the industrial—community. In addition, this facility is providing an increasingly unique resource for the characterization and preservation of protein crystals grown in the microgravity environment.

RESEARCH APPROACH

Protein crystallography is currently the most powerful method for the determination of the three-dimensional structure of proteins and other macromolecules. This method usually requires crystals which are relatively large (0.5 mm to 1.0 mm) in size and possess a reasonably high degree of internal order. Consequently, protein crystal growth has become the subject of an increasing number of fundamental studies in crystal growth, including several ongoing microgravity experiments.

The knowledge of the three-dimensional structure of macromolecules is of fundamental importance to the field of molecular biology, and it is presently receiving considerable attention from the biotechnology industry, based on its promising potential for application in rational drug design and protein engineering. This year we have successfully augmented the diffraction laboratory to include a new imaging plate detector system, significantly expanding our scientific capabilities. In addition to the evaluation of the X-ray diffraction properties of protein crystals, this laboratory is utilized to determine the three-dimensional structures of several challenging problems in molecular biology.

Crystals of several important proteins have been grown in our laboratory, including a new crystal form of HSA. *Chalaropsis* lysozyme, cytochrome c5, the Fab portion of the antibody expressed against gp41 of the human immunodeficiency virus (HIV-1), and Interleukin 6. HSA is the most abundant protein of the circulatory system. There it plays several major roles in the transport, distribution, and metabolism of a diverse variety of endogenous and exogenous ligands. The three-dimensional structure of HSA was determined for the first time in our laboratory in 1989. The detailed atomic structure will provide a wealth of information regarding the many remarkable properties of this protein.

Chalaropsis lysozyme is an enzyme which displays a broad-spectrum bacteriolytic function and apparently belongs to a novel lysozyme structural class. A detailed understanding of this molecular structure will explain the chemical basis of the bacteriolytic function and could provide important information for future experiments in biotechnology. The crystals of cytochrome c5 diffract X-rays to very high resolution (approximately 1.0 angstroms) and will provide further insight into the mechanisms of electron transport. The structure of the HIV Fab will reveal important information concerning antibody/antigen interaction and offers additional insight into the design of new recombinant therapeutic antibodies. The structure determination and refinement of these and other protein crystals is actively in progress.

PROGRESS DURING FY1992

The structure of HSA has been successfully determined and refined to a resolution of 2.8 angstroms. The results were published this year in a major research article in the journal *Nature*. Crystals of several other serum albumins with enhanced quality have been successfully grown in our laboratory over the past year as well. Many cocrystallization complexes have been successfully grown with a variety of long-chain fatty acids. These crystals promise to provide further insight into the important area of albumin research.

Our laboratory was involved in support of several Spacelab missions during the 1992 time frame (IML-1, USML-1, and SL-J). Preliminary assessments of the quality

of HSA crystals grown in microgravity (IML-1) have revealed significant enhancements in the resolution and number of observed diffraction data for selected crystals, providing the best crystal of the HSA form grown to date. Recombinant HSA, wild-type HSA, and an antibody fragment expressed against the HIV-1 virus (from our laboratory) flew, together with approximately 25 other proteins, on USML-1 PCG. However, our proteins failed to crystallize, for some as yet undetermined reason. Further investigations of the difference between ground-based and flight crystals will be addressed pending additional flight opportunities.

The atomic coordinates obtained from the HSA crystallographic studies are now being applied to understand the detailed chemistry of serum albumin. Additionally, several other serum albumin structures have now been determined by the molecular replacement method to better than 3.0 angstrom resolution; among these is the recently refined structure, sequence, and chemistry of horse serum albumin. Some of these structures are still in the refinement stage until the complete amino acid sequences have been determined. Comparisons of these structures are revealing a wealth of information regarding the evolution and chemistry of these important macromolecules. Further details of these studies will be published in the near future.

The three-dimensional structure of a human monoclonal antibody (Fab 3D6), which binds specifically to the transmembrane protein gp 41 of the human immunodeficiency virus type 1 (HIV-1), has been determined by crystallographic methods of 2.7 angstroms. The antibody belongs to the subclass IgG1 (kappa) and exhibits antibody-dependent cellular cytotoxicity.

The quaternary structure of the Fab is in an extended conformation with an elbow bending angle between the constant and variable domains of 175 degrees. Hypervariable loop H3, residues 102H to 109H, is unusually extended from the surface. The complementarity-determining region forms a hydrophobic pocket that is created primarily from hypervariable loops L3, H3, and H2. Studies with a small antigenic peptide suggest that this binding pocket recognizes the putative solvent exposed disulphide loop CSGKLIC of gp 41.

Although numerous Fab structures have now been determined by crystallographic methods, this is the first representative structure of a human monoclonal antibody and the first structure of a human antibody expressed against a major epitope of the AIDS virus. This structural work is part of series which aims to elucidate the detailed nature of human monoclonal antibodies expressed against the AIDS virus together with their respective antigenic complexes. This work has now been published in the *Proceedings of the National Academy of Science.*

The high-resolution structure of cytochrome c5 is currently under refinement at 1.35 angstroms. This work is now being conducted in conjunction with the NASA JOVE

program through collaboration with Prof. Ross Reynolds and is proceeding according to expectations.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

— DeLucas, L. J., Smith, C. D., Ealick, S. E., Carter, D. C., Twigg, P., He, X. M., Snyder, R. S., Weber, P. C., Schloss, J. V., Einspahr, H. M., Clancy, L. L., McPherson, A., Koszelak, S., Vandonselaar, M. M., Prasad, L. Quail, J. W., Delbaere, L. T. J., and Bugg, C. B. Protein crystal growth aboard the U.S. Space Shuttle Flights STS-31 and STS-32. *Proceedings of the committee on Space Research (COSPAR) XXVIII Plenary Meeting, The Hague, the Netherlands. Advances in Space Research,* vol. 12, No. 1, 393-400 (1992).

— He, X. M., and Carter, D. C. The three-dimensional structure of a novel lysozyme from *Chalaropsis*. Manuscript in preparation, 1992.

— He, X. M., and Carter, D. C. Atomic structure and chemistry of human serum albumin. *Nature 358,* 209–215 (1992).

— He, X. M., Ruker, F., Casale, E., and Carter, D. C. The structure of a human monoclonal antibody against gp 41 of the human immunodeficiency virus type 1. *Proceedings of the National Academy of Science, USA 89,* 7154–7158 (1992).

— Miller, T. Y., He, X. M., and Carter, D. C. A comparison between protein crystal grown with vapor diffusion methods in microgravity and protein crystals using a gel liquid-liquid diffusion method. *J. Crystal Growth, 122,* 306–309 (1992).

TYPE: Ground
DISCIPLINE: Protein Crystal Growth
PROJECT TITLE: *Protein Crystal Growth in Low Gravity*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-23-08-19

PRINCIPAL INVESTIGATOR: Dr. Robert S. Feigelson
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TASK OBJECTIVE/DESCRIPTION

The ultimate objective of this research program is the careful design of an experiment to study the effect of low gravity on the growth of protein crystals in a long-duration space flight. The proper design of the flight hardware and experimental protocols are highly dependent on understanding the factors which influence the nucleation and growth of crystals of biological macromolecules. Thus, the primary objective of this research is centered on investigating these factors and relating them to the body of knowledge which has been built up for "small molecule" crystallization. These data also provide a basis of comparison for the results obtained from low-g experiments.

RESEARCH APPROACH

This research program was designed to study the mechanisms of protein crystal growth and the parameters which influence growth and crystal perfection. Canavalin was chosen as a model protein in initial studies which included (a) a determination of its solubility diagram, (b) a study of the growth rate of canavalin crystals, (c) a determination of the growth mechanism, and (d) a study of the fluid flow behavior around growing protein crystals. These tasks have been completed and published.

The current scope of the program has been directed toward other protein materials, including lysozyme and isocitrate lyase, and toward new processing techniques designed to control nucleation and growth independently. This part of the program now includes the following subjects:

1. Determination of the relationship between gravity and the morphology and quality of isocitrate lyase crystals (this involves determining the factors which cause isocitrate lyase to grow as dendritic crystals in 1-g and as more equi-axed crystals in μg);

2. Development of a method for controlling the nucleation and growth processes independently through the use of localized supersaturation control;

3. Development of a predictive model for protein crystal growth;

4. Development of conceptual designs for long-term space flight experiments based on the data gathered by this program; and

5. Development of an understanding of the relationship between growth rate and crystal perfection.

PROGRESS DURING FY1992

The previous nucleation studies with the Thermonucleator used materials with a known temperature dependence of solubility. In addition, these materials (ice water, Rochelle salt, and lysozyme) exhibit normal crystallizing (solubility) behavior, meaning that they crystallize when the temperature is lowered. To further test the capabilities of the Thermonucleator, two proteins with retrograde solubility (solubility that increases with decreasing temperature) were used: horse serum albumin (HSA) and α chymotrypsinogen A (αCA). The nucleation of retrograde protein posed the potential problem of a strong fluid flow being induced by the warm nucleation probe at the bottom of a cooler solution. While flows were observed, they did not interfere with the nucleation process or cause the nuclei to move away from the probe. The crystallizing solutions were based on the work of McPherson for HSA (McPherson, *Preparation and Analysis of Protein Crystals*, Wiley, 1982, p. 128) and Matthews, *J. Mol. Biol. 33*, 1968, p. 499). The solutions were placed in the apparatus and the temperatures adjusted to produce nucleation. The HSA nucleated at a probe temperature of 29 °C and an ambient of 16 °C; the αCA at a probe temperature of 20 °C and an ambient of 9 °C. No attempt was made to optimise the nucleation conditions for either protein.

The original Thermonucleator is too large to be of use in the μg environment, It also relies on water circulation for control of the ambient temperature and liquid nitrogen to provide cooling for the nucleation probe. Neither of these is compatible with operation on either the orbiter or the space station. A new Thermonucleator has been designed which uses thermoelectric elements to provide temperature control. This unit measures 10.2 cm x 7.5 cm x 7.5 cm. It is designed to fit into a rack which will provide power, temperature sensing and control, cooling for the thermoelectric elements, and light for illuminating the growing crystal. This apparatus is currently being built.

One of the problems that has plagued any scheme for controlling the nucleation phase of crystal growth is the detection of nucleation. A system has been designed to use static light scattering to detect nucleation on the nucleation probe. This system will be installed on the original Thermonucleator for testing purposes.

Recent work by Durbin has shown that it is possible to image the surface of growing protein crystals using atomic force microscopy (AFM). The Center for Materials Research has recently acquired a second generation AFM unit that has a potential resolution of 10Å or less. This will allow us to image individual protein molecules as they enter the crystalline lattice. We have begun the basic studies that will allow us to study the crystallization of proteins under a variety of conditions and relate the formation of defects to the growth conditions.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— DeMattei, R. C., and Feigelson, R. S. Controlling nucleation in protein solutions. *J. Crystal Growth, 122,* 21 (1992).

— DeMattei, R. C., Feigelson, R. S., and Weber, P. C. Factors affecting the morphology of isocitrate lyase crystals, *J. Crystal Growth, 122,* 152 (1992).

— Feigelson, R. C. "Factors affecting the morphology of isocitrte lyase crystals." International Conference on Crystal Growth, San Diego, CA, August 1992.

— Feigelson, R. C. "Thermal methods in protein crystallization." International Conference on Crystal Growth, San Diego, CA, August 1992.

TYPE: Ground
DISCIPLINE: Protein Crystal Growth
PROJECT TITLE: *Studies on the Protein Crystal Nucleation Process*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** 674-23-08-16

PRINCIPAL INVESTIGATOR: Dr. Marc L. Pusey
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TASK OBJECTIVE/DESCRIPTION

The objective was to study the initial stages of protein crystal nucleation using the protein hen-egg lysozyme as a model. We wanted to determine the onset of aggregation under saturated solutions and the extent of aggregation in supersaturated solutions.

RESEARCH APPROACH

The primary techniques to be developed and used were light scattering intensity and isothermal calorimetry. Another technique, dialysis kinetics, which by passed many of the theoretical and practical limitations of light scattering, was developed and is now being refined. As phase data is vital to understanding these processes, continuous development and use of a rapid solubility technique was done.

Results from the above experiments have led us to the conclusion that any understanding of the initial events in protein crystal nucleation must encompass an understanding of the role played by the precipitating species, in this case the Cl-ion. This has led to the development of a fluorescence technique for measuring the interactions of Cl with protein.

PROGRESS DURING FY1992

The project has been completed. While the initial goals have not been fully met, this is because their solution has required us to investigate ever more fundamental questions about the protein desolubilization process. A complete phase diagram of one crystalline form (tetragonal) of lysozyme has been determined, while that of a second (orthorhombic) is now approximately 80% finished. Overall, all data indicated that the protein is much more aggregated both in over- and under-saturated solutions, than previously believed. Further, this aggregation must affect the mechanism of crystal growth.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Cacioppo, E., and Pusey, M. L. The solubility of the tetragonal form of hen egg white lysozyme from pH 4.0 to 5.4. *J. Crystal Growth, 114* 286–292 (1992).

— Cacioppo, E., Munson, S., and Pusey, M. L. Protein solubilities determined by a rapid technique and modification of that technique to a micro-method. *J. Crystal Growth, 110*, 66–71 (1991).

— Forsythe-Cacioppo, E., and Pusey, M. L. The effects of acid treatment and calcium ions on the solubility of concanavalin A. *J. Crystal Growth, 122*, 208–212 (1992).

— Pusey, M. L. Estimation of the initial equilibrium constants in the formation of tetragonal lysozyme nuclei. *J. Crystal Growth, 110*, 60–65 (1991).

— Pusey, M. L. Continuing adventures in lysozyme crystal growth. *J. Crystal Growth, 122*, 1–7 (1992).

— Pusey, M. L., and Munson, S. Micro-apparatus for rapid determination of protein solubilities. *J. Crystal Growth, 113*, 385–389 (1991).

— Wilson, L. J., and Pusey, M. L. Determination of monomer concentrations in crystallizing lysozyme solutions. *J. Crystal Growth, 122*, 8–13 (1992).

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Noncontact Temperature Measurements*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: Ali Abtahi
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TASK OBJECTIVE/DESCRIPTION

The objective is to continue the development of a variety of noncontact techniques to accurately sense small temperature changes in high-temperature furnace applications.

RESEARCH APPROACH

An additional temperature-sensing technique was conceptualized which will be developed in the coming year.

PROGRESS DURING FY1992

In 1992 continued studies have been made utilizing the Division of Amplitude Polar Pyrometer. Applications include better high temperature-measurement and data-acquisition capability for materials-processing studies.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Thomas, A. S. W. Correction-free radiometry of specular spheres for containerless processing in microgravity. Accepted by 1992.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Microwave Furnace Development*
RESPONSIBLE CENTER: JPL **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: Dr. Martin B. Barmatz
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PHONE: (818) 354-3088

TASK OBJECTIVE/DESCRIPTION

The goal of this project is to develop a high efficiency, cold wall, direct-heating microwave furnace. Such a furnace will allow direct and rapid heating of microwave-absorbing materials. It is expected that directed heating zones will be able to be created, thereby providing more versatility to the furnace process control. An added advantage derived from the use of a direct heating furnace is that rapid cooling is possible upon removal of the microwave energy source.

RESEARCH APPROACH

Focused energy from various microwave sources has been used to conduct material melt and resolidification studies.

PROGRESS DURING FY1992

Various energy-level studies conducted on a selected group of materials have resulted in successful melting of the specimens. Development of furnace microwave tuning techniques was also begun. As a result of this novel furnace technology, an entirely new approach to furnace processing techniques may occur.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Barmatz, M. Microwave processing materials in microgravity. *Proceedings of the First Technical Interface Meeting for the Modular Containerless Processing Facility, 2,* 262, (1992).

— Barmatz, M. B. and Jackson, H. W. Steady state temperature profile in a sphere heated by microwaves. *MRS Microwave Processing of Materials III, 269, 97,* (1992).

— Barmatz, M., Watkins, J. L., and Jackson, H. W. "Microwave processing of materials in microgravity." 30th Aerospace Sciences Meeting and Exhibit, AIAA Paper #92-0116, January 1992.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Ultrasonic Interface Measurements of Crystal Growth*
RESPONSIBLE CENTER: LaRC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: Dr. Archibald L. Fripp
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TASK OBJECTIVE/DESCRIPTION

Noncontact sensing and shape quantification of the solid/liquid interface of high-temperature crystal growth processes is being made possible. This capability will provide the potential for a real-time feedback measurement to control a crystal-growth process.

RESEARCH APPROACH

Two methods bring investigated are the time-of-flight and pulse-echo techniques. The former requires two transducers, one at either end of the sample, while the latter has the advantage of only requiring a single measurement location.

PROGRESS DURING FY1992

In 1992, the ability to transmit and receive ultrasonic pulses from a high-temperature sample was successfully demonstrated. Refinements to this pulse-echo technique are now in progress.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Carter, J. N., Lam, A., and Schleich, D. M. Ultrasonic time-of-flight monitoring of the position of the liquid/solid interface during the Bridgman growth of germanium. *J. Scientific Instruments*; vol. 63, p. 3472, 1992.

— Hubert, J. A., Fripp, A. L., and Welch, C. S. Numerical thermal analysis of a sample of germanium with a centerline capillary tube in a vertical Bridgman furnace. In preparation for *J. Crystal Growth* 1992.

PATENTS — Fripp, Archibald L. "Real-Time Ultrasonic Melt-Solid Interface Measuring Device." Case # LAR 14877-1-CU.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Microgravity Fluids and Combustion Diagnostics*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** Not Applicable

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TASK OBJECTIVE/DESCRIPTION

The success in achieving a significant scientific return from existing and proposed microgravity fluid physics and combustion science experiments depends substantially on the availability of diagnostic systems for the collection of the required scientific data.

Currently, the available diagnostic instrumentation for achieving these objectives has been extremely limited, consisting primarily of conventional film-based imaging systems and intrusive temperature and velocity probes, such as thermocouples and hot wire anemometers. This situation has arisen primarily because of the unique and severe operational constraints which are inherent in the conduct of reduced-gravity experimentation. It is the recognition of this pressing need to provide diagnostic systems of greater sophistication that has motivated the existence of this particular development program.

RESEARCH APPROACH

For a variety of reasons, predominant emphasis has been placed on the development of optical diagnostic techniques. Principal among these is the relative fragility of the physics and chemistry of reduced-gravity systems relative to their 1-g counterparts. The action of buoyancy-induced convection is vigorous when compared with the dominant mechanisms associated with reduced-gravity phenomena, such as surface tension and thermal and concentration driven diffusion processes. The essentially nonperturbative nature of optical measurement techniques is therefore extremely appropriate in this context.

Optical measurement techniques are, in general, well-suited to the acquisition of multidimensional data fields (e.g., two- and three-dimensional imaging). This is an important consideration in the present state of understanding of microgravity science, since a clearer understanding of basic phenomenology, including the verification of fundamental length and time scales and dominating physical mechanisms in still being developed.

PROGRESS DURING FY1992

The determination of refractive index fields has long been utilized as a method for the qualitative visualization of combustion reaction. Quantification of the refractive index distribution can frequently be used to determine temperature distributions or relative species concentrations in nonreacting flows.

For the purposes at hand, interferometric methods are not ideally suited, owing principally to their severe requirements for mechanical stability. Deflectometric methods, such as Schlieren and Moore, tend to be far less complex, more tolerant to mechanical and thermal fluctuations, and readily adaptable to large fields of view.

The system that has been developed is based on the use of continuously graded colored rainbow filters. The qualitative appearance of the observed images affords a vast amount of detail, owing to the eye's ability to resolve fairly subtle differences in color. In addition, the continuous nature of the color filter represents a distinct advantage over conventional knife-edge methods from the standpoint of spatial resolution. Furthermore, it has been demonstrated that a reasonably simple image digitization and processing system can be used to quantify the color attributes of the observed image, and hence the refractive index distribution which produced it. Present results indicate that comparable sensitivity to conventional interferometry has been achieved. The ability to quantitatively determine the resulting ray deflections has been completed and is in the process of submittal for publications. This system has subsequently been employed to measure refractive index distribution in radiantly heated liquid pools, axially symmetric jet diffusion flames, and solid surface combustion.

A system of this type has been constructed for reduced gravity tests in the 2.2-second drop tower facility. It is based on a breadboarded configuration that has been utilized in the laboratory. A support service contractor has provided the engineering, design, and fabrication support for the overall design and construction of the final system. The set of tasks for which they were responsible includes a dedicated drop package incorporating a number of features which will be useful in the subsequent implementation of additional diagnostic experiments. The optical and electronic subsystems have been integrated and tested. Reduced gravity tests are anticipated to commence by year's end.

An improved optical configuration, as well as the fabrication and testing process, have been designed. Unlike the previous configuration, which utilizes off-axis parabolic primary mirrors, this configuration employs spherical primaries. Spheric surfaces are considerably less costly to fabricate, a significant consideration when constructing a system with a reasonably large field of view (the initial version of the spheric system provides a 150 mm FOV). The use of spheric surfaces introduces other aberrations, however, which must then be corrected by subsequent optical elements. These additional elements have been suitably designed to achieve the required corrections while simultaneously providing net angular magnification.

This angular magnification is necessary to meet the original design goal of providing a long effective focal length system (3000 mm) in a relatively small package (550 mm). This configuration has been incorporated into a KC-135 package which has been flown in three campaigns since January 1992.

Planar (i.e., two-dimensional) imaging of Rayleigh scattering has been reported by numerous investigators for the determination of gas-phase density distribution. The application to actual flames is, however, hindered by the presence of relatively strong naturally occurring broad-band emissions. It seems unlikely that the continuous wave (CW) sources presently available in the laboratory will be able to overcome this aspect of the problem.

By utilizing a pulsed source with a synchronously gated detector, the strength of the scattered signal relative to the strength of the emission lines can be satisfactorily reduced. The FY1992 effort focused on the determination of the pulse energies that are required, and the identification of a pulsed laser diode array commensurate with these requirements. Such an array would be compact enough to be utilized in an aircraft or drop-tower configuration. In addition, the tunable solid-state laser system slated for procurement during FY1992 is ideally suited for this application.

The chemistry of the formation of soot and the substantial heat loss due to radiation motivate an increased understanding of the role of soot in microgravity combustion phenomena. Specifically, the mass fraction and size distribution are desirable quantities to determine experimentally. Experiments are being conducted in the laboratory using transmission (i.e., absorption), scattering, and sampling techniques. The principal investigator (PI) for these experiments is Dr. J. C. Ku from Wayne State University. Dr. Ku is presently supported under grant as a result of the most recent NASA Research Announcement (NRA) for microgravity combustion.

The determination of size and concentration requires the simultaneous measurement of two quantities. In this case, transmission measurements are accompanied by either the collection of soot samples, or by an additional scattering measurement. These techniques have been successfully conducted in the laboratory, and have since been incorporated into a 2.2-second drop package. The initial configuration accommodates full-field absorption measurements using a low power laser source, and a thermophoretic sampling probe. In the latter, extremely small wire electron microscopy grids are rapidly inserted in to the flame and withdrawn (total residence time of approximately 30 milliseconds). The size distribution of the soot particles is then analyzed from scanning electron micrographs.

A suitably constructed sampling probe has been constructed so as to minimally perturb the flames upon insertion and withdrawal. High-speed photography and high Schlieren imaging have been performed to validate the essentially nonintrusive nature of the probe. The particle-size distribution information is then

used to compute an effective per-particle absorption cross section. This allows the absorption data to be inverted to obtain soot number densities. These inversions have been successfully performed using data obtained under normal gravity conditions, and they agree well with published values. Reduced-gravity experiments have shown much larger sizes for both primary particles and aggregates. These results are presently being prepared for publication.

Laser Doppler Velocimetry (LDV) is a nonintrusive optical technique for the accurate determination of point-wise velocity data. In some instances, it is possible to perform line or area scans before the flowfield was evolved significantly. Recent development in solid-state laser diode and avalanche photodiode detector technologies have made available LDV systems which are quite compact (65 mm diameter, 130 mm length), and require only a few watts of electrical power. Arrangements have recently been made to procure a device of this type. This will form the basis for a complete LDV system, which includes data acquisition and signal processing electronics, optics for implementing line and are a scans, and a seeding system for introducing scattering particles into the flow stream.

Although the vendor is capable of producing a hardened version suitable for use in

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Buchele, D. R. and Griffin, D. W. A compact color Schlieren optical system. Accepted for publication in *Applied Optics.*, 1992.

— Weiland, K. J. Intensified array camera imaging of solid surface combustion aboard the NASA Learjet. Accepted for publication in *Proceedings of the AIAA 30th Aerospace Sciences Meeting, 6th Annual Space Proceeding Conference,* Reno NV, January 6–9, 1992.

— Greenberg, P. S. "Constraints and capabilities of combustion diagnostics in Microgravity." Second International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

— Weiland, K. J. "Visualization and imaging methods for flames in microgravity." Second International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

— Griffin, D.W. "Selected microgravity combustion diagnostic techniques." Second International Microgravity Combustion Workshop, Cleveland, OH, September 15–17, 1992.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Advanced Furnace Technology*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: Dr. Sandor L. Lehoczky
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TASK OBJECTIVE/DESCRIPTION

The task objective is to assess the effectiveness of transverse and axial magnetic fields for suppressing gravity induced fluid flows during the directional solidification of selected semiconducting alloys. The objective also involves the development of methods using magnetic fields for the management and control of potential deleterious effects associated with the presence of varying levels of steady and time dependent residual acceleratons and possible surface tension gradient driven flows.

RESEARCH APPROACH

The research approach is to evaluate furnace concepts using a superconducitng magnet up to 5 Tesla by developing heater element concepts for use in a high magnetic field, designing, fabricating, and testing a furnace module for magnetic field use that simulates the thermal characteristics of the Crystal Growth Furnace and has the translation range capabilities suitable for the currently identified AADSF and CGF experiments. The approach also involves performing crystal growth experiments to evaluate the effects of axial magnetic fields and evaluating concepts for shielding of stray magnetic fields.

PROGRESS DURING FY1992

A CGF-like furnace was installed in the 5 Tesla superconducting magnet, tested, and brought into full operating condition. All subsystems including translation, temperature control, and a mechanical pulser were integrated. The heater windings in the hot zone were upgraded to platinum/rhodium wire. Gallium-doped germanium samples have been grown to test the furnace. A ceramic permanent magnet was constructed with a shielding assembly and the fields inside and outside the assembly were measured.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Stereo Imaging Velocimetry*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: Dr. Mary Jo B. Meyer
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TASK OBJECTIVE/DESCRIPTION

Stereo imaging velocimetry will permit the collection of quantitative, three-dimensional flow data from any optically transparent fluid which can be seeded with tracer particles. This includes such diverse experiments as the strudy of multiphase flow, bubble nucleation and migration, pool combustion, and crystal growth, all of which are part of NASA's microgravity science program.

The objectives of this project are to develop a stereo imaging velocimeter which will (a) measure fluid velocities between 1.0 mm/sec and 10.0 cm/sec with an accuracy of +1.0% for 150-micron seed particles in a 3.0-cm field of view, (b) have streamlined data processing which processes 100 time steps of consecutive stereo images to obtain 3-D velocity fields in ten minutes or less, (c) be able to track at least 100 particle pairs per frame, (d) require minimal a priori assumptions about the flow, and (e) initiate tracking and matching without human intervention.

RESEARCH APPROACH

Our approach to successful implementation is to choose the most promising of current techniques as our starting point, and develop or modify algorithms to accomplish particle centroid finding, tracking, and matching, as well as camera calibration. These four capabilities are the basis for the velocimeter and will determine its final processing speed and accuracy. We will then test the prototype for accuracy on particles moving in known trajectories. User interface for both the front-end and postprocessing will be created. The velocimeter will be tested on real fluid experiment(s).

PROGRESS DURING FY1992

During 1992 we chose two promising methods (already in existence in the literature) on which to build our stereo imaging velocimeter. One method, which uses fast-scan particle recognition and probability trees for tracking and matching, was

coded under a subcontract at Ohio State University and delivered to our laboratory at the end of FY92.

The second method, which uses a boundary-tracking particle recognition scheme and a geometrical particle tracking or matching scheme with back checking for errors, is currently being coded in our lab (Bethea). Camera calibration has been investigated in great detail (Meyer) and the code for the three best methods was duplicated. We have begun to examine neural nets as an alternative camera calibration scheme, because current camera calibration methods generally address only two-dimensional scenes.

GRADUATE STUDENTS: 2 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Meyer, M. B., and Bethea, M. D. "A Full Field, 3-D velocimeter for NASA's microgravity science program." 30th Aerospace Sciences Meeting & Exhibit
Reno, NV, January 6–9, 1992.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: ***Laser Light Scattering Instruments***
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: William V. Meyer
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TASK OBJECTIVE/DESCRIPTION

The objective is to develop sturdy, miniaturized laser light scattering instrumentation and operational software.

RESEARCH APPROACH

Thie task is using state-of-the-asrt fiberoptic technology in a building-block fashion to create modular and versatile subsystems and systems.

PROGRESS DURING FY1992

This year (FY92), the single-angle detector system was delivered and evaluations have begun. Also, advances have been made in the use of back-scatter probes in studies of nontransparent solutions. Applications are as diverse as sensing nucleation and diffusion and studies of cataracts.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 2

PUBLICATIONS/PRESENTATIONS

— Ansari, R. R., Dhadwal, H. S., Campbell, M. C. W., and Dellavecchia, M. A. Fiber optic sensor for opthalmic refractive diagnostics. In *Fiber Optic Medical and Fluorescent Sensors and Applications* , vol. 1648, pp. 83–105, in *Progress in Biomedical Optics,* A. Katzir, ed., SPIE Publication, 1992.

— Ansari, R. R., Dhadwal, H. S., Cheung, H. M., and Meyer, W. V., "A fiber optic probe for the characterization of microemulsions." 9th International Symposium on Surfactants in Solution, Paper # Sn3.D1.2, Varna, Bulgaria, June 10–15, 1992.

— Ansari, R. R., Dhadwal, H. S., Cheung, H. M., Meyer, W. V. "Microemulsion characterization using a fiber optic probe." Photon Correlation and Scattering (Theory and Applications), Paper # MA5, 8th Topical Meeting, Optical Society of America, Morgantown, West Virginia, August 24–26, 1992.

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— Rim, Y. H., Cawley, J. D., Ansari, R. R., and Heyer, W. V. In-situ light scattering study of aggregations. *Ceramic Transactions: Forming Science and Technology for Ceramics.* M. J. Cima, ed. vol. 26, 1992.

— Ross, D. A., and Dhadwal, R. S. Regularized inversion of the Laplace transform: Accuracy of analytical and discrete inversion. *Particle Systems Characterization 8*, 282–286, (1991).

— Meyer, W. V., and Ansari, R. R. A preview of a microgravity laser light scattering instrument. *AIAA* , 91-0779, January 1991.

— Ansari, R. R. and Meyer, W. V., "Static and dynamic laser light scattering studies of series 78 nylon 6,6 Polymer." NASA/DuPont Confidential Divisional Report, April 1991.

— Ansari, R. R., and Meyer, W. V., "Laser light scattering studies on the interactions and characterization of alumina and pliolite plastic particles in silicone oil." Space Experiment Division Technical Report, NASA-LeRC, April 1991.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Surface Light Scattering Instruments*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: William V. Meyer
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TASK OBJECTIVE/DESCRIPTION

The objective is the development of an instrument capable of detecting fluid surface phenomena, such as local temperatures and interface temperature gradients, surface tensions, and volume viscosity.

RESEARCH APPROACH

We started with an Argon ion pumped grating heterodyne surface-light-scattering spectrometer. Our equipment has developed to the state where the bulk optics/high power/large space requirements of the traditional surface-light system have been replaced by a low-power compact laser-diode-pumped surface-light-scattering system.

Development of an autotracking surface light-scattering spectrometer that can also measure surface physical parameters within a small localized surface domain is underway. This optically self-stabilizing spectrometer is now being tested. This work is being extended by the use of fiber optics and incorporation of acousto-optic modulators that will detect surface gradients. The design phase of measuring the high-amplitude surface ripplons is nearing completion.

PROGRESS DURING FY1992

Initial work accomplished has included surface-light-scattering data collection, using laboratory systems, and development of the theoretical equations to accomplish measurements on curved surfaces.

GRADUATE STUDENTS: 1   **DEGREES GRANTED:** 0

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Multizone Transparent Furnace*
RESPONSIBLE CENTER: LeRC **PROJECT IDENTIFICATION:** Not Applicable

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TASK OBJECTIVE/DESCRIPTION

The objective was to determine the ability to create a controllable multizone furnace while still providing a view of the sample being processed. Technology development resulted in demonstration of the ability to develop and build a working transparent, multizone-controlled modular furnace system for use in materials-processing experiments.

RESEARCH APPROACH

Various video imaging processes were applied and evaluated to determine the sample interface shape.

PROGRESS DURING FY1992

Development of a multizone transparent furnace was concluded.

GRADUATE STUDENTS: 1 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Batur, C., Sharpless, R. B., Duval, W. M. B., and Rosenthal, B. N., Self-tuning multivariable pole placement control of multizone crystal growth furnace. *Journal of Adaptive Control and Signal Processing*, vol. 6, pp. 111–123, 1992.

— Batur, C., Sharpless, R. B., Duval, W. M. B., and Rosenthal, B. N., "Self-tuning multivariable pole placement control of multizone crystal growth furnace." Presented at The Winter Annual Meeting of the ASME, Control of Manufacturing Processes, Altanta, GA, December 1–6, 1991, DSC-Vol. 28, PED-Vol. 52.

— Batur, C., Sharpless, R. B., Duval, W. M. B., Rosenthal, B. N., and Singh, N. B., Identification and control of a multizone crystal growth furnace. *Journal of Crystal Growth, 119*, pp. 371–380, (1992).

— Rosenthal, B. N. "Advanced technology development program review: transparent furnace technology." Presented at the ATD Program Review, Washington DC, May 5, 1992.

TYPE: ATD
DISCIPLINE: Not Applicable
PROJECT TITLE: *Multicolor Holography*
RESPONSIBLE CENTER: MSFC **PROJECT IDENTIFICATION:** Not Applicable

PRINCIPAL INVESTIGATOR: William K. Witherow
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TASK OBJECTIVE/DESCRIPTION

A noncontact method of simultaneously determining concentration and temperature variations in fluid systems is underway. An additional benefit will be the additional simultaneous data- acquisition capability and thus a possible reduction in the number of experiment runs required per mission.

RESEARCH APPROACH

In this system, two fluid parameters will be varied simultaneously, and this technique will measure the variations by using two different frequency lasers. More complete multivariable research on fluid science experiments will be enabled by this new capability.

PROGRESS DURING FY1992

Confirmation of the capability to measure fringe lines to sufficient resolution was made this year (FY92). This capability will now provide the ability to continue with full measurement system development.

GRADUATE STUDENTS: 0 **DEGREES GRANTED:** 0

PUBLICATIONS/PRESENTATIONS

— Trolinger, J. D., Lal, R., Vikram, C. S., and Witherow, W. K. Compact space flight solution crystal growth system. *Proceedings SPIE*, vol. 1557, 250–258, 1991.

— Vikram, C. S., and Witherow, W. K. Critical needs of fringe-order accuracies in two-color holographic interferometry. *Experimental Mechanics*, March 1992, 74–77.

— Vikram, C. S., Witherow, W. K., and Trolinger, J. D. Refractive properties of TGS acqueous solution for two-color interferometry. *Proceedings SPIE*, vol. 1557, 197–201, 1991.

— Vikram, C. S., Witherow, W. K., and Trolinger, J. D. Special beam intensity ratio needs in multicolor holography. Submitted to *Journal of Modern Optics* November 1992.

III.
Microgravity Science & Applications Bibliography for FY 1992

How to Order Publications Cited in this Document

Copies of many documents cited in the bibliography given herein are available from the Center for AeroSpace Information (CASI), a NASA Scientific and Technical Information (STI) Program facility. Prices are determined by the number of pages of each document and whether paper or microfiche copy material is ordered.

NASA Center for AeroSpace Information (CASI)
P.O. Box 8757
Baltimore, MD 21240-0757
Telephone: (301) 621-0390
FAX: (301) 621-0134

FLIGHT

Flight: Biotechnology

Mukherjee, P., and Hymer, W. C. Heterogeneity of rat pituitary prolactin cells: Relationships among location, hormone assay and estrous cycle stage. *Neuroendocrinimmunology,5*, 108–119, (1992).

Mukherjee, P., Epp, L., Viselli, S., Mastro, A. M., and Hymer, W. C. "PRL cell function in the individual rat pituitary gland in vitro: Importance of physiological state of the donor." Presented at the 74th Annual Meeting of the Endocrine Society, 1992.

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Viselli, S., and Mastro, A. M. PRL receptors are found on a heterogeneous subpopulation of rat splenocytes. *Endocrinology*. In press, 1992.

Flight: Combustion Science

Altenkirch R. A., Bhattacharjee, S., Olson, S. L., and Sacksteder, K. "Opposed-flow flame spreading in reduced gravity." 2nd International Microgravity Combustion Workshop, Cleveland, OH, September 15-17, 1992.

Altenkirch, R. A., Tang, L., Bullard, D. B., and Bhattacharjee, S. "Unsteady flame spread over solid fuels in microgravity." Presented by R. A. Altenkirch at the World Space Congress, Washington, DC, September 5, 1992.

Bahadori, M.Y., and Edelman, R. B. Combustion of gaseous fuels under reduced-gravity conditions. Paper LB-038, *Proceedings of the Second Symposium on Lunar Bases,* Lunar and Planetary Institute, Houston, Texas, in press, 1992.

Bahadori, M. Y., Edelman, B., Stocker, D. P., Sotos, R. G., and Vaughan, D. F. "Effects of oxygen concentration on radiative loss from normal-gravity and microgravity flames." Paper AIAA-92-0243, AIAA 30th Aerospace Sciences Meeting, Reno, NV, January 1992.

Bahadori, M. Y., Stocker, D. P., Vaughan, D. F., Zhou, L., and Edelman, R. B. "Effects of buoyancy on laminar, transitional, and turbulent gas jet diffusion flames." Presented at the Second International Microgravity Combustion Workshop, Cleveland, OH, September 1992.

Bahadori, M. Y., Vaughan, D. F., Stocker, D. P., Weiland, K. J., and Edelman, R. B. "Preliminary observations on the effects of buoyancy on transitional and turbulent diffusion flames." Presented at the 1992 Spring Technical Meeting of the Central States Section of the Combustion Institute, Columbus, OH, April 1992.

Bhattacharjee, S., Altenkirch, R. A., and Sacksteder, K. Implications of spread rate and temperature measurements in flame spread over a thin fuel in a quiescent, microgravity, space-based environment. In preparation for *Combustion Science and Technology*, 1992.

Bhattacharjee, S., and Altenkirch, R. A. A comparison of theoretical and experimental results in flame spread over thin condensed furls in a quiescent, microgravity environment. *Proceedings of the Twenty-fourth Symposium (International) on Combustion,* Sydney, Australia. In preparation, 1992.

Bhattacharjee, S., Bhaskaran, K. K. and Altenkirch, R. A. "Effects of pyrolysis kinetics on opposed-flow flame spread modeling." Presented by S. Bhattacharjee at the ASME/AIChE National Heat Transfer Conference, San Diego, CA, August 8–12, 1992.

Bhattacharjee, S., Seaton, D., and Altenkirch, R. A. "The role of kinetic, transport, and thermodynamic properties on flame spread over a thin solid fuel in an opposed flow environment." Presented by D. Seaton at the Western States Section of the Combustion Institute meeting, Berkeley, CA, October 12–13, 1992, WSSCI Paper no. 92-107.

Buckmaster, J. B., Gessman, R., and Ronney, P. D. "The three-dimensional dynamics of flame balls." Twenty-Fourth International Symposium on Combustion, Sydney, Australia, July 1992.

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Dryer, F. L. "Computational/experimental studies of isolated, single-component droplet combustion." Presented at the Second International Microgravity Combustion Workshop, NASA Lewis Research Center, Cleveland, OH, October 1992.

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Fernandez-Pello, A. C., and Pagni, P. J. "A fundamental study of smoldering combustion in microgravity." Presented at the Second International Microgravity Combustion Workshop, NASA LeRC, September 1992.

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Shy, S. S., Ronney, P. D., Buckley, S. G., and Yakhot, V. "Experimental simulations of premixed turbulent combustion using aqueous autocatalytic reactions." Twenty-Fourth International Symposium on Combustion, Sydney, Australia, July 1922.

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Torero, J. L., Kitano, M., and Fernandez-Pello, A. C. Opposed forced flow smoldering of polyurethane foam. Accepted for publication by *Combustion Science and Technology*, 1992.

West, J., Bhattacharjee, S., and Altenkirch, R. A. "Investigation of controlling parameters in transition between thermally thin and thermally thick flame spread over solid fuels in an opposing flow." Presented by J. West at the Western States Section of the Combustion Institute meeting, Berkeley, CA, October 12–13, 1992, WSSCI Paper no. 92-106.

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Williams, F. A. "Studies of droplet burning and extinction." Presented at The Second International Microgravity Combustion Workshop, NASA Lewis Research Center, Cleveland, OH, October 1992.

Flight: Electronic Materials

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Appendix

APPENDIX A: TABLE OF ACRONYMS

The following list of acronyms, though by no means complete, includes those used in this document as well as some that are often found in text associated with Microgravity Science and Applications research and which may be encountered when reviewing references cited in the bibliography herein.

AADSF	Advanced Automated Directional Solidification Furnace
AAL	Aero-acoustic Levitation
ACRT	Accelerated Crucible Rotation Technique
AO	Announcement of Opportunity
AOMS	Advanced Optical Monitoring Systems
APCF	Advanced Protein Crystallization Facility
APCG	Advanced Protein Crystal Growth
ATD	Advanced Technology Development
BTF	Biotechnology Facility
CADAP	Computer-Aided Dendrite Analysis Program
CASTE	Casting and Solidification Technology Experiment
CBE	Chemical Beam Epitaxy
CCD	Charge-coupled Device
CFLSE	Critical Fluid Light Scattering Experiment
CFTE	Critical Fluid Thermal Equilibration Experiment
CFVME	Critical Fluid Viscosity Measurement Experiment
CGF	Crystal Growth Furnace
CNES	Centre Nationale d'Études Spatiales [The French National Center for Space Studies]
CoDR	Conceptual Design Review
CPF	Critical Point Facility
CSA	Canadian Space Agency
CVD	Chemical Vapor Deposition
CVTE	Chemical Vapor Transport Experiment
CW	Continuous Wave
DARA	Deutsche Agentur für Raumfahrtangelegenheiten [German Space Agency]
DLR	The German Aerospace Research Establishment
DPM	Drop Physics Module

DSC	Differential Scanning Calorimetry
DSF	Directional Solidification Furnace
DTA	Differential Thermal Analysis
EDM	Engineering Development Model
EDS	Energy Dispersive Spectroscopy
EHD	Electrohydrodynamic
ESA	European Space Agency
FDSMM	Fluid Dynamics and Solidification of Metallic Melts
FES	Fluids Experiments System
FES/VCGS	Fluid Experiment/Vapor Crystal Growth System
FFEU	Free-Flow Electrophoresis Unit
GaAs	Gallium Arsenide
GAS Can	Get-away Special Canister
GBX	Glovebox
GFFCE	Geophysical Fluid Flow Cell Experiment
GJDFE	Gas Jet Diffusion Flames Experiment
HMO	Heavy Metal Oxide
HRT	High-Resolution Thermometer
ICARUS	Integrated Convection Apparatus and Rotating Undercarriage Support
ICE	Interface Configuration Experiment
IDGE	Isothermal Dendritic Growth Experiment
IML	International Microgravity Laboratory
IWG	Investigator Working Group
JOVE	Joint Ventures
JPL	Jet Propulsion Laboratory
JSC	Johnson Space Center
KSC	Kennedy Space Center
LaRC	Langley Research Center
LDV	Laser Doppler Velocimetry
LeRC	Lewis Research Center

LPE	Lambda Point Experiment
MEPHISTO	Matériel pour l'Étude des Phenomènes Intéressants de la Solidification sur Terre et en Orbite [Interesting Phenomena of Solidification on Earth and in Orbit]
MGM	Mechanics of Granular Materials
MGM	Microgravity Measurement
MMSL	Microgravity Materials Science Laboratory
MP	Microgravity Pressure
MPa	Microgravity Pressure, Ambient
MSA	Microgravity Science and Applications (Program)
MSAD	Microgravity Science and Applications Division
MSFC	Marshall Space Flight Center
MSL	Microgravity Science Laboratory
NASA	National Aeronautics and Space Administration
NASDA	National Space Development Agency of Japan
NIST	National Institute for Standards and Technology
NLO	Nonlinear Optical
NRA	NASA Research Announcement
NRC	National Research Council
OMCVD	Organometallic Chemical Vapor Epitaxy
OPCGA	Observable Protein Crystal Growth Apparatus
OSSA	Office of Space Science and Applications
PBE	Pool Boiling Experiment
PCG	Protein Crystal Growth
PDA	Phase Doppler Pneumometer
PIV	Particle Image Velocimetry
PMZF	Programmable Multizone Furnace
POCC	Payload Operations Control Center (at MSFC)
PVT	Physical Vapor Transport
RAPIV	Radiographic Particle Image Velocimetry
RDR	Requirements Definition Review

RPCVD	Remote Plasma-enhanced Chemical Vapor Epitaxy
RSD	Rainbow Schlieren Deflectometry
RTE	Radiative Transfer Equation
RTOP	Research and Technology Operations Places
SAA	South Atlantic Anomaly
SAMS	Space Acceleration Measurement Systems
SCE	Smoldering Combustion Experiment
SCF	Supercritical Fluid
SEM	Scanning Electron Microscopy
SL	ESA Spacelab (in Space Shuttle cargo bay; e.g., IML and USML)
SQUID	Superconducting Quantum Interference Detector
SSCE	Solid Surface Combustion Experiment
SSF	Space Station *Freedom*
SSFF	Space Station Furnace Facility
STDCE	Surface Tension Driven Convection Experiment
STEP	Space Technology Experiments Platform
STS	Space Transportation System
SVP	Space Vehicle Pressure
TEM	Transmission Electron Microscopy
TEMPUS	Electromagnetic Containerless Processing Facility
TME	Test and Measurement Equipment
TMS	Thermal Maneuvering System
USML	United States Microgravity Laboratory
USMP	United States Microgravity Payload
USRA	Universities Space Research Association
VCGS	Vapor Crystal Growth System
VDA	Vapor Diffusion Apparatus
XRD	X-ray Diffraction

APPENDIX B: INDEX TO PRINCIPAL INVESTIGATORS

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The tasks are grouped into three categories appropriate to the type of research being done-space flight, ground based, and advanced technology development-and by science discipline. The science disciplines are: biotechnology, combustion science, electronic materials, fluid physics, fundamental physics, glass and ceramics, metals and alloys, and protein crystal growth.

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